Chemistry in young gas-rich disks: overview

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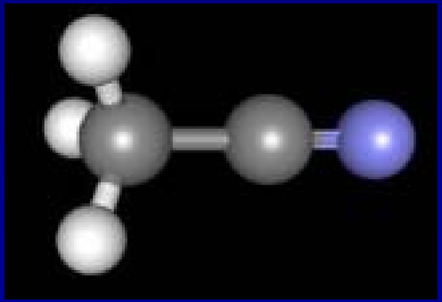
Leiden Observatory



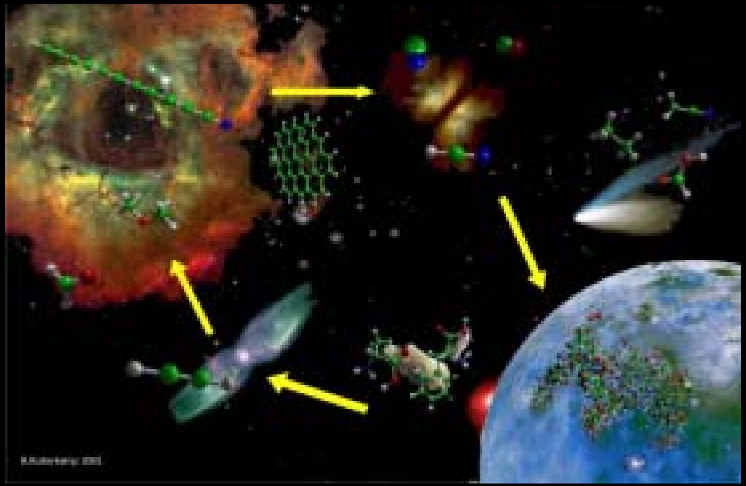
Outline

- Observations
  - Single-dish submillimeter
  - Millimeter interferometry
  - Infrared spectroscopy
    - absorption toward edge-on disks
- Models
  - Radial transport models
  - 1+1D, 2D models of static flaring disks
  - Tenuous ‘transitional’ disks
- Summary

Discuss only outer disk chemistry 50-400 AU

Why chemistry?

- **Detection of exoplanets => renewed interest in inventory and lifecycle gas + dust**
  - **Is chemical composition interstellar or 'nebular'? How is it modified in disks?**
- **Molecules as probes of disk structure**
  - **Radial + vertical T, n, ionization fraction, ….**
- **Chemistry as tracer of dynamical processes**
  - **Degree of vertical mixing?**
- **Molecules as tracers of gas mass**
  - **When does gas disappear?**



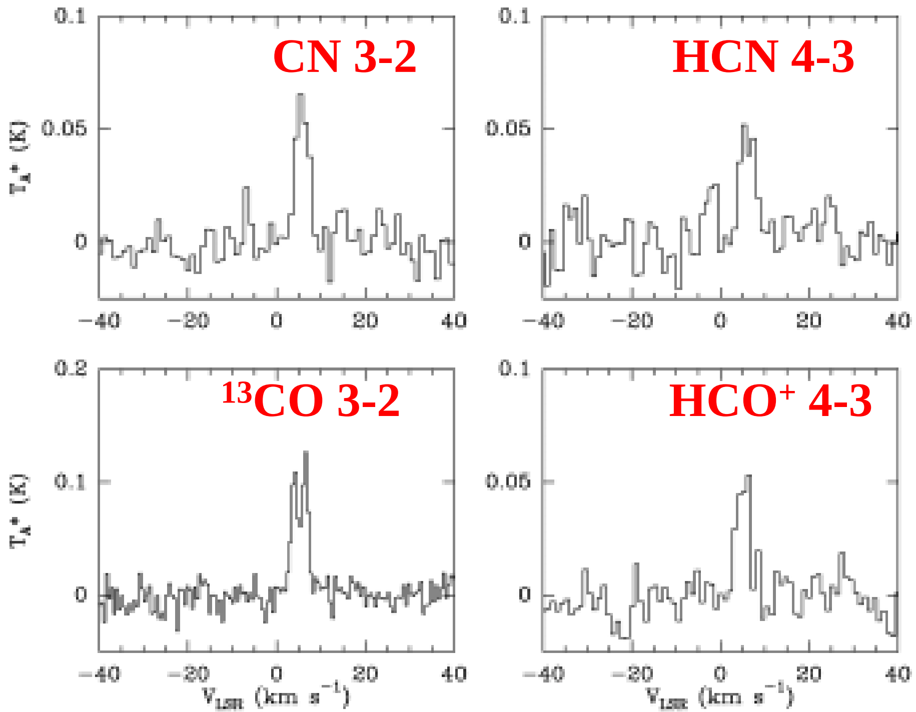
I. Observations: submillimeter single dish

- Observations of molecules other than CO
  - Initial detections by Dutrey et al. 1997, Kastner et al. 1997
  - Subsequent surveys by van Zadelhoff et al. 2001, Thi et al. 2004, Greaves 2004, Bacmann, Schreyer et al. in prep, ….
- Advantage high-frequency => high-J lines
  - Critical densities well matched to high densities in disks
    - Probe n=10^6-10^8 cm^{-3}, T=10-100 K
  - Smaller beams at high frequency => less beam dilution
    - 10-15” => data are spatially unresolved for disks at 150 pc
  - Avoid confusion with any surrounding cloud or envelope material
    - M_{disk}~0.01 M_{sun}, 100 times less than typical protostellar envelope mass

Lines are weak: at limit of capabilities current facilities!

Examples single-dish data

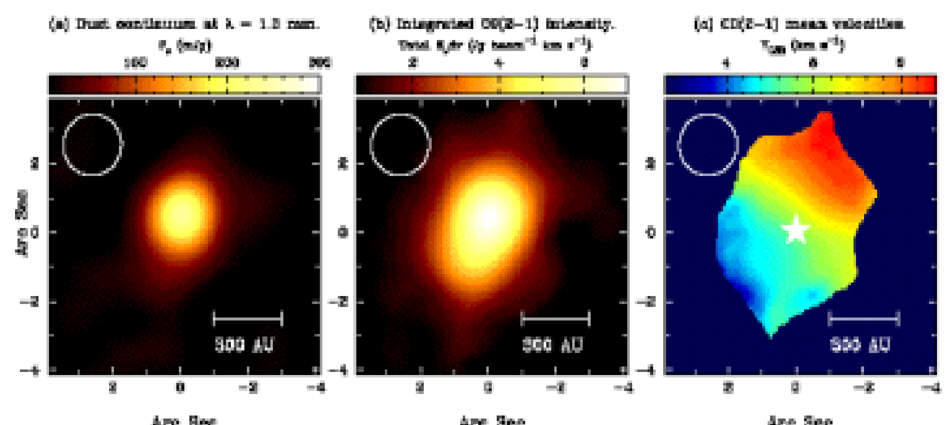
JCMT



LkCa 15:
T Tauri star

MWC 480:
Herbig Ae star

Thi et al. 2004

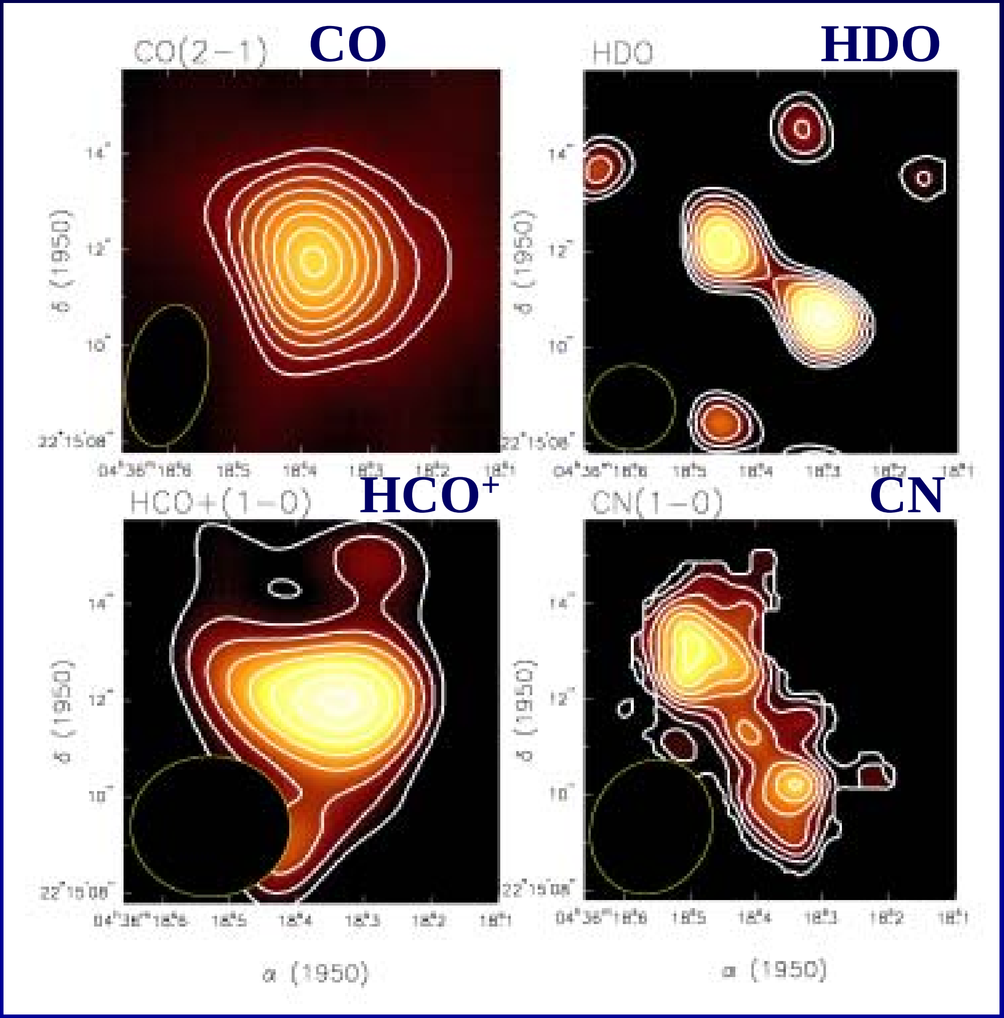


MWC 480
OVRO

Mannings & Sargent 1997

Observations: millimeter interferometry

Starting to image the chemistry on 100 AU scales



LkCa 15:
OVRO mm array
2” resolution

Kessler, Qi, Blake et al. 2003

See also: Aikawa et al. 2003, Dartois et al. 2003

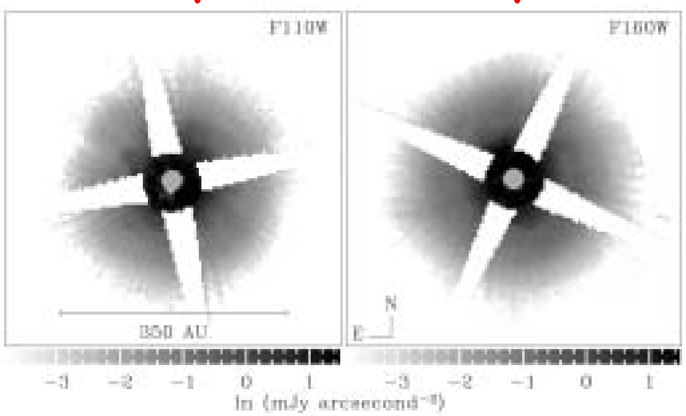
Some observational findings: submillimeter data

- Simple gas-phase molecules observed
  - Ion-molecule reactions (HCO^+, N_2H^+)
  - Photo-processes (high CN/HCN)
  - High deuterium fractionation (DCO^+, H_2D^+)
  - Few complex organic species detected (H_2CO, CH_3OH)
- Data only sensitive to >50 AU
- Lines come from ‘warm’ 20-40 K layer with $n=10^6$-10^8 cm^{-3}
- Disk-averaged abundances are ‘depleted’ by factor of 5-100
  - Using mass from dust continuum and assuming gas/dust=100
- Molecules can have different radial distributions
  - E.g., HCN and CN inner ‘hole’, in contrast with CO and HCO^+

Detection of DCO^+ in the TW Hya disk

TW Hya face-on disk

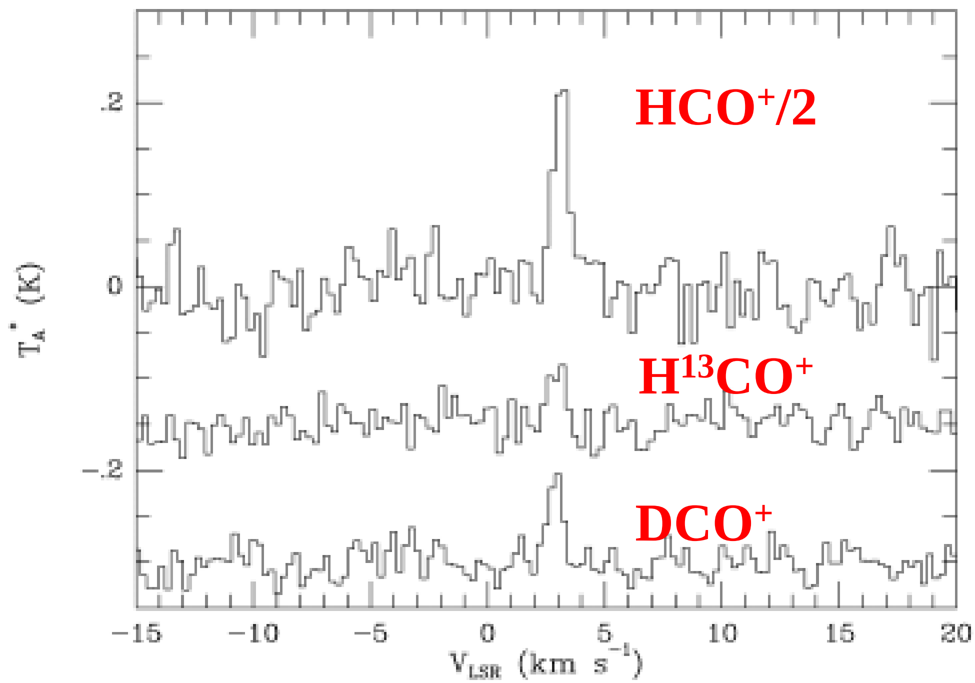
1.1 μm   1.6 μm



Scattered light => radius 200 AU

Weinberger et al. 2002

JCMT



van Dishoeck et al. 2003

- **$DCO^+/HCO^+=0.035$ => emission arises from layer with heavy depletions**
- **Level of deuterium fractionation comparable with that found in cold pre-stellar cores and comets**
- **HCO^+ abundance few x 10^{-11} – 10^{-10} => lower limit on ionization fraction**

Origin of strong deuteration

$$H_3^+ + HD \rightleftharpoons H_2D^+ + H_2$$

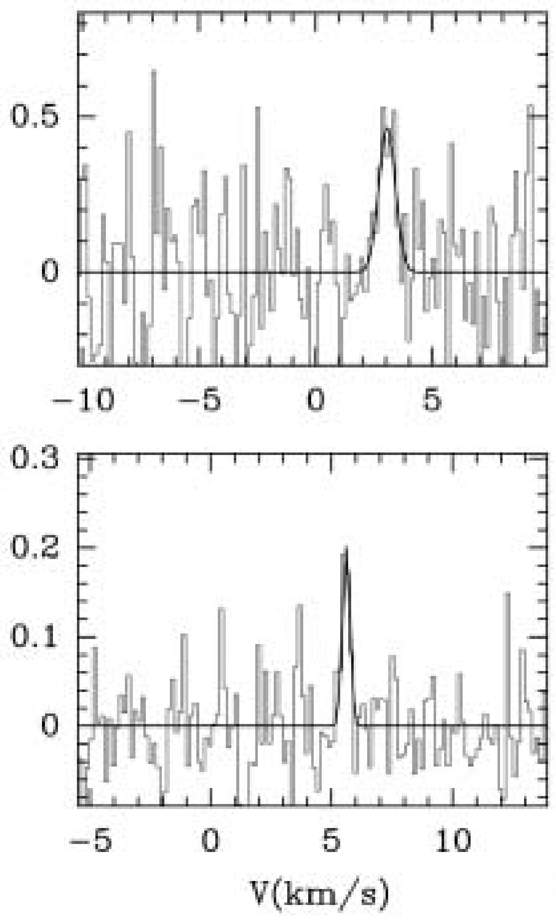
$$H_2D^+ + X \rightleftharpoons XD^+ + H_2$$

- Reactions more rapid in forward direction at low T
- H_3^+ and H_2D^+ greatly enhanced when their main destroyer, CO, is frozen out on grains

=> H_2D^+ should be best probe of cold midplane!

Detection of H_2D^+ in disks

Measuring the ionization degree in the midplane



TW Hya
CSO data

DM Tau

-Inferred ionization fractions at least few times 10^{-10} => sufficient for MRI mechanism to operate

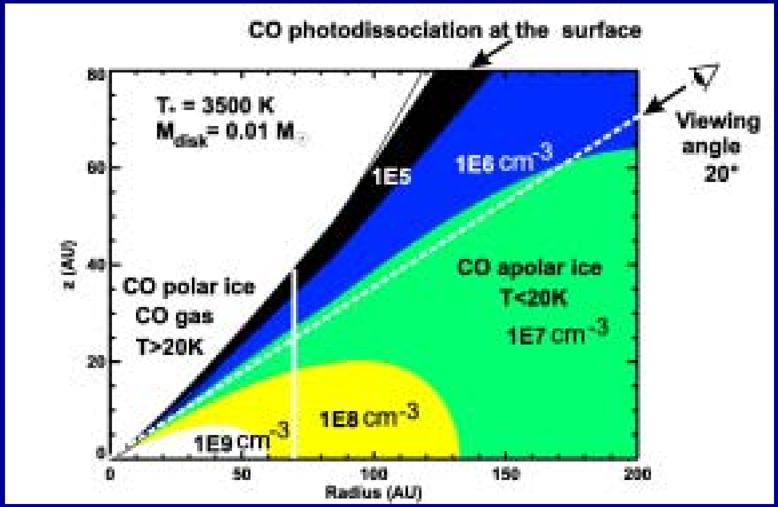
Ceccarelli et al. 2004

Infrared vs submillimeter

- **Submillimeter:**
  - **Very high spectral resolution (R>10^6, <0.1 km/s)**
  - **Many gas-phase molecules with abundances down to 10^{-11} w.r.t. H_2**
  - **Emission => radial distribution at high angular resolution**
- **Infrared:**
  - **Moderate spectral resolution (R~10^3-10^4)**
  - **Gases *and* solids with abundances down to 10^{-7}-10^{-8}**
  - **Molecules without permanent dipole moments (H_2, C_2H_2, CH_4, CO_2, CH_3, …)**
  - **PAHs, silicates, ices**
  - **Absorption => pencil beam line-of-sight**

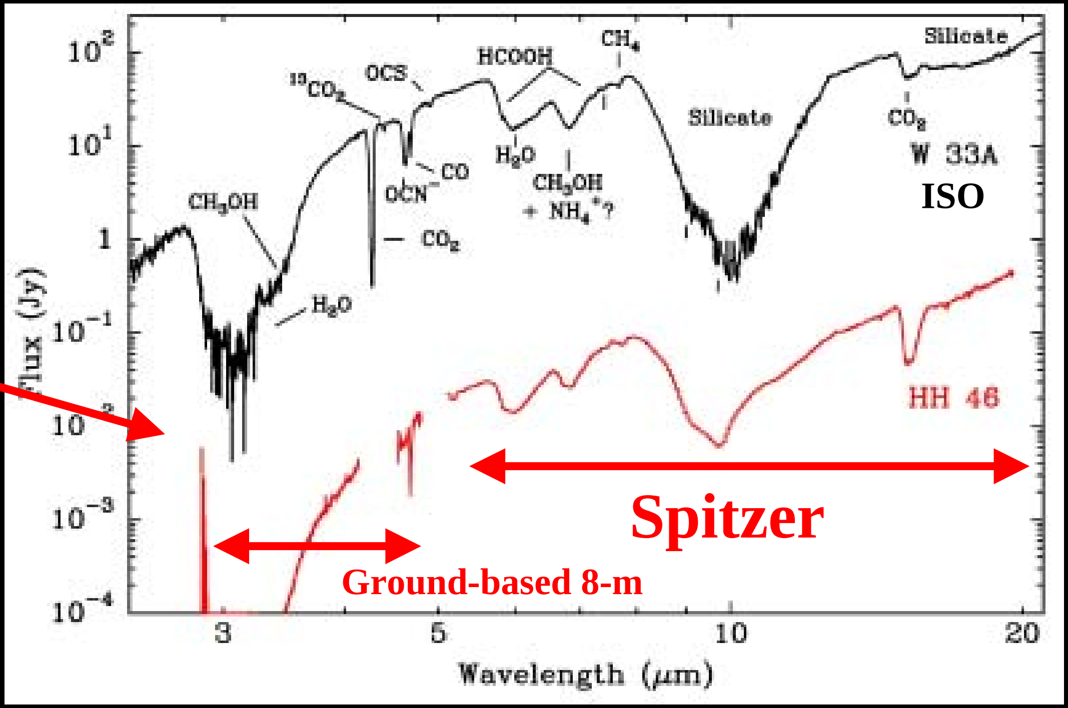
Observations: infrared spectroscopy

- Emission in vibrational bands of H_2, CO, H_2O, H_3^+ (TBC) => warm gas in inner few AU
  - Weintraub et al. 2001, Brittain & Rettig 2002, Brittain et al. 2003, Najita et al. 2003, Carr et al. 2003, Blake & Boogert 2004
- Silicate + PAH emission => see later talks
- Absorption of gases + ices toward edge-on disks



Spitzer's potential for ice observations

HH 46: solar-mass YSO

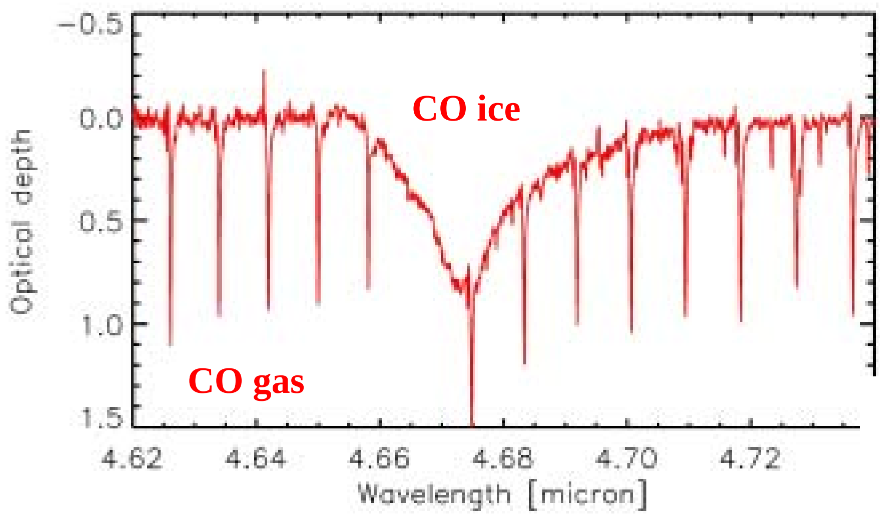


- Spitzer can study objects >100 times fainter than ISO
- Ice absorptions originate in cold outer envelope
- Abundances similar to high-mass YSO's, but higher solid CO_2 abundance up to CO_2/H_2O=0.4
- Evidence for thermal processing up to 50 K

Noriega-Crespo et al. 2004
Boogert et al. 2004

Ices toward a young, large edge-on disk

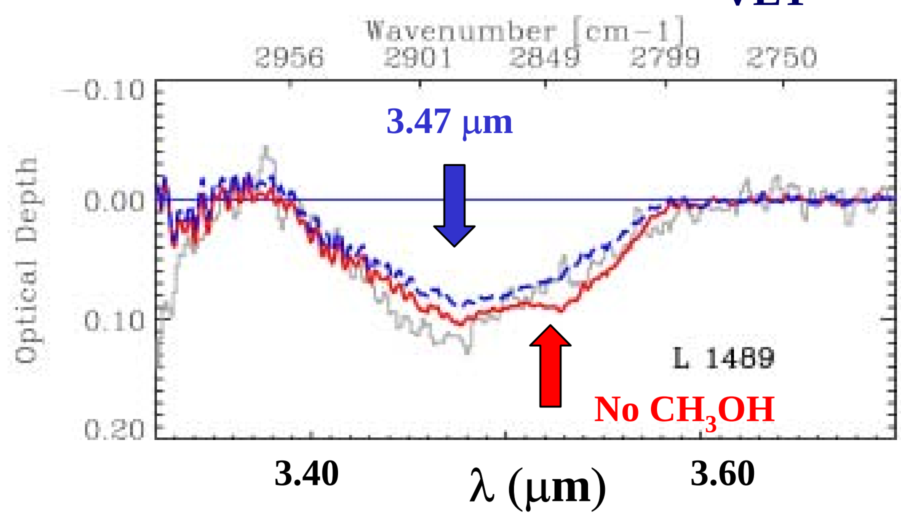
L1489 Taurus



Keck

R=25,000

VLT

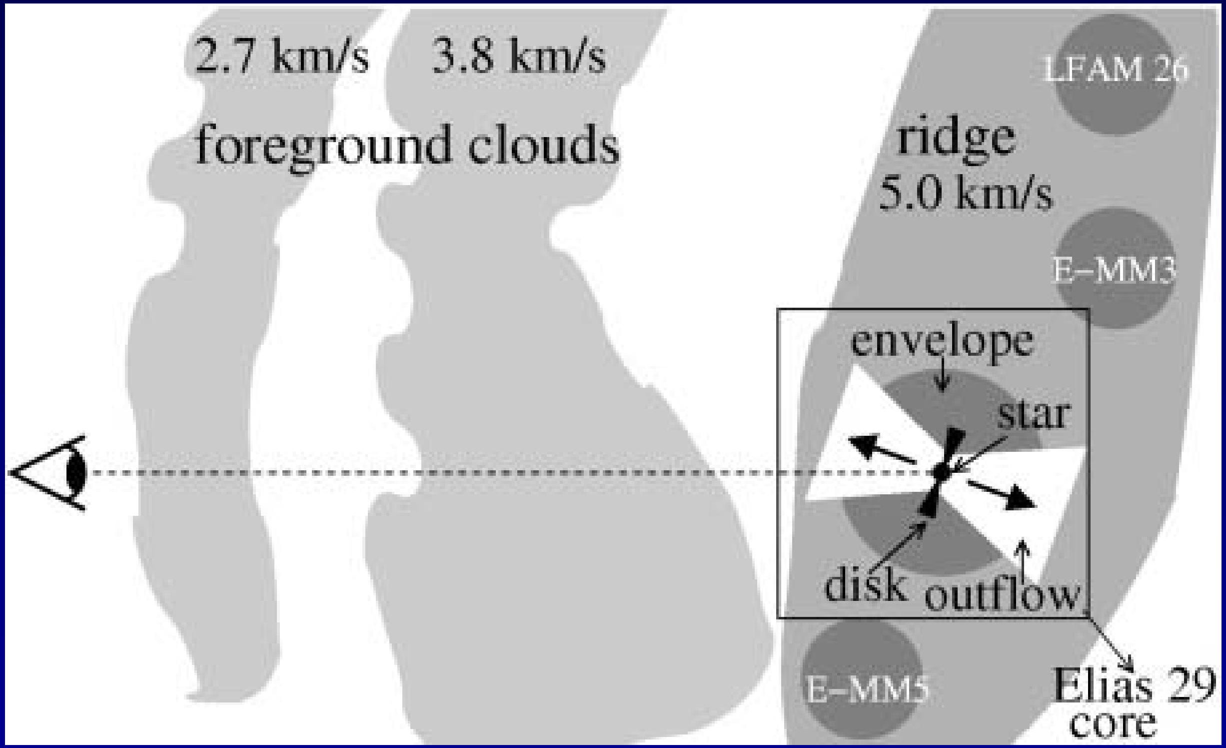


- Warm CO gas with CO_{gas}/CO_{solid}~10
- No CH_3OH ice, key ingredient for making complex organic molecules CH_3OH/H_2O<5%
- Significant fraction of ices outside disk?

Boogert, Hogerheijde & Blake 2002
Pontoppidan et al. 2003

See also: Shuping et al. 2001 Elias 18

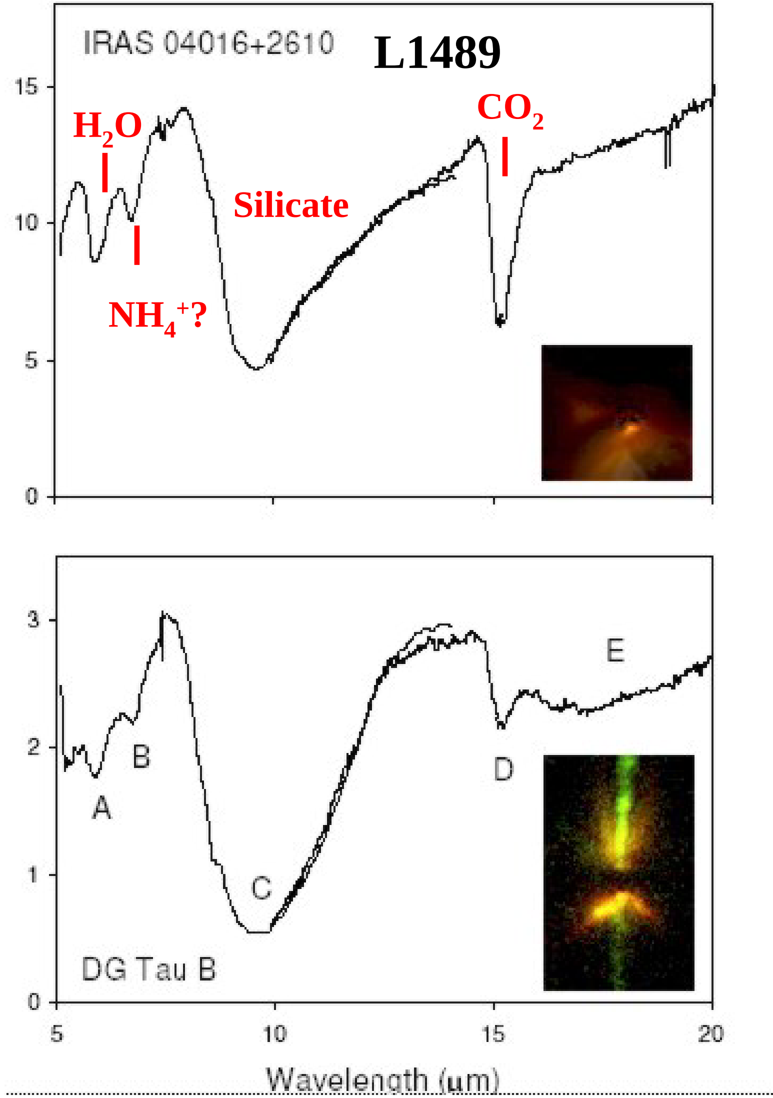
Where are the ices along the line-of-sight?



- Significant fraction of ice absorption can arise in foreground clouds and/or envelopes => need detailed study of each object individually
- Geometry very important

Boogert et al. 2001

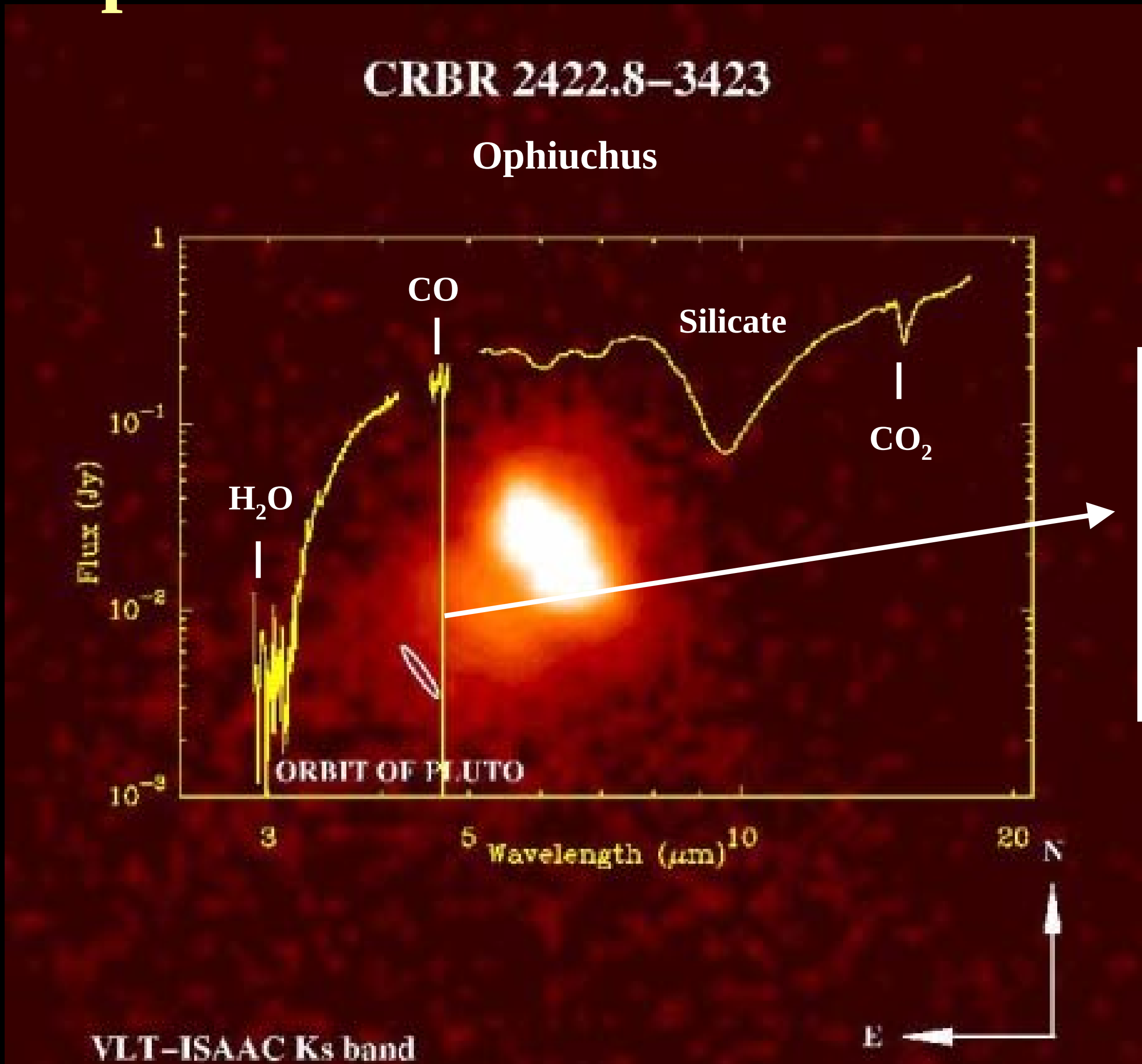
Spitzer observations of edge-on disks



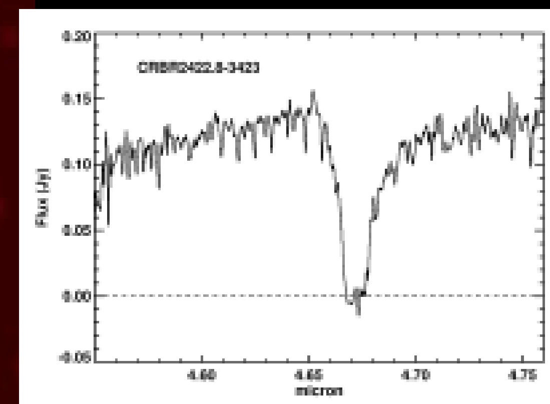
- Ices may arise primarily in outer envelope

Watson et al. 2004

Spitzer + VLT observations of edge-on disk



Strongest solid CO absorption ever observed!

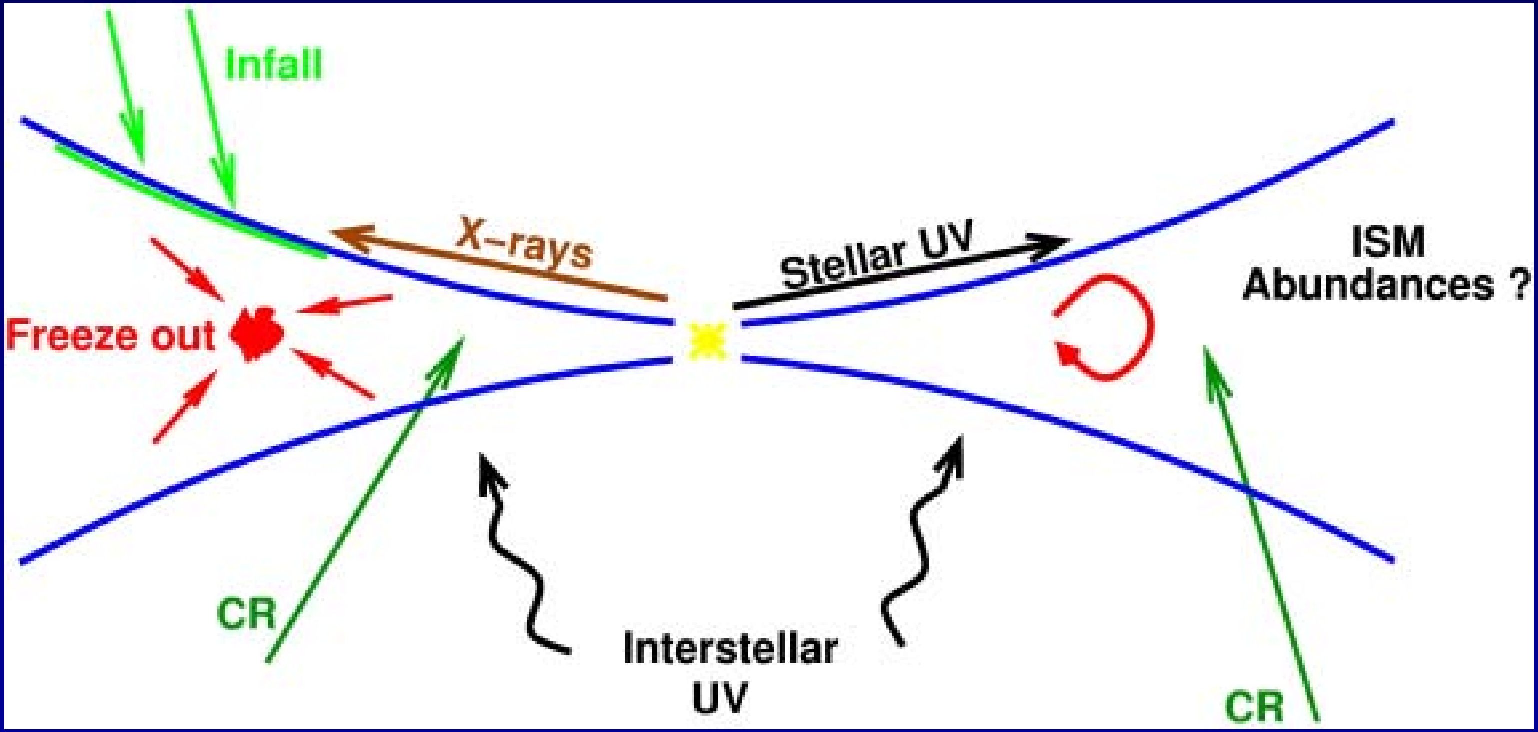


CO_{solid}/CO_{gas}~1
$T_{ex}(CO)$~50 K

Thi et al. 2002
Pontoppidan, Dullemond et al. 2004

-- Abundances w.r.t. H_2O ice similar to low-mass YSO envelopes
- Detailed modeling of disk + surroundings indicates that up to 50% of ice absorptions may arise in disk; ices in disk may be heated to >40 K

II. Models: chemical processes in disks



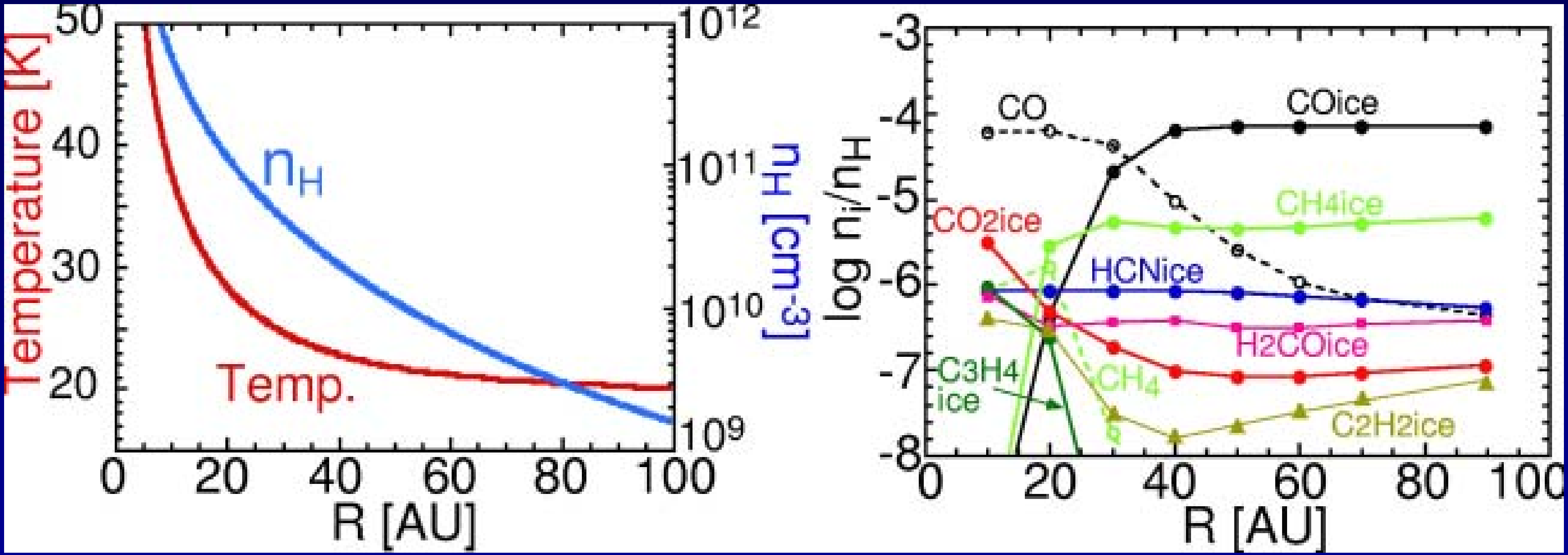
Focus on outer disk chemistry, i.p. effect of UV

1D radial transport models

- Consider chemical evolution of parcel of gas as it moves radially from >100 AU to few AU
- Include large gas-phase chemistry network (few hundred species, few thousand reactions) and gas-grain adsorption/desorption processes
- Chemistry dominated by temperature profile: virtually no gas-phase molecules >10 AU, active gas-phase chemistry <10 AU
  - E.g., Bauer et al. 1997, Finocchi & Gail 1997, Gail 2001-2004, Willacy et al. 1998, Aikawa et al. 1997, 1999

Example

Abundances after $3x10^6$ yr, disk midplane



=> Everything frozen out at >10 AU

But this is NOT what is observed!

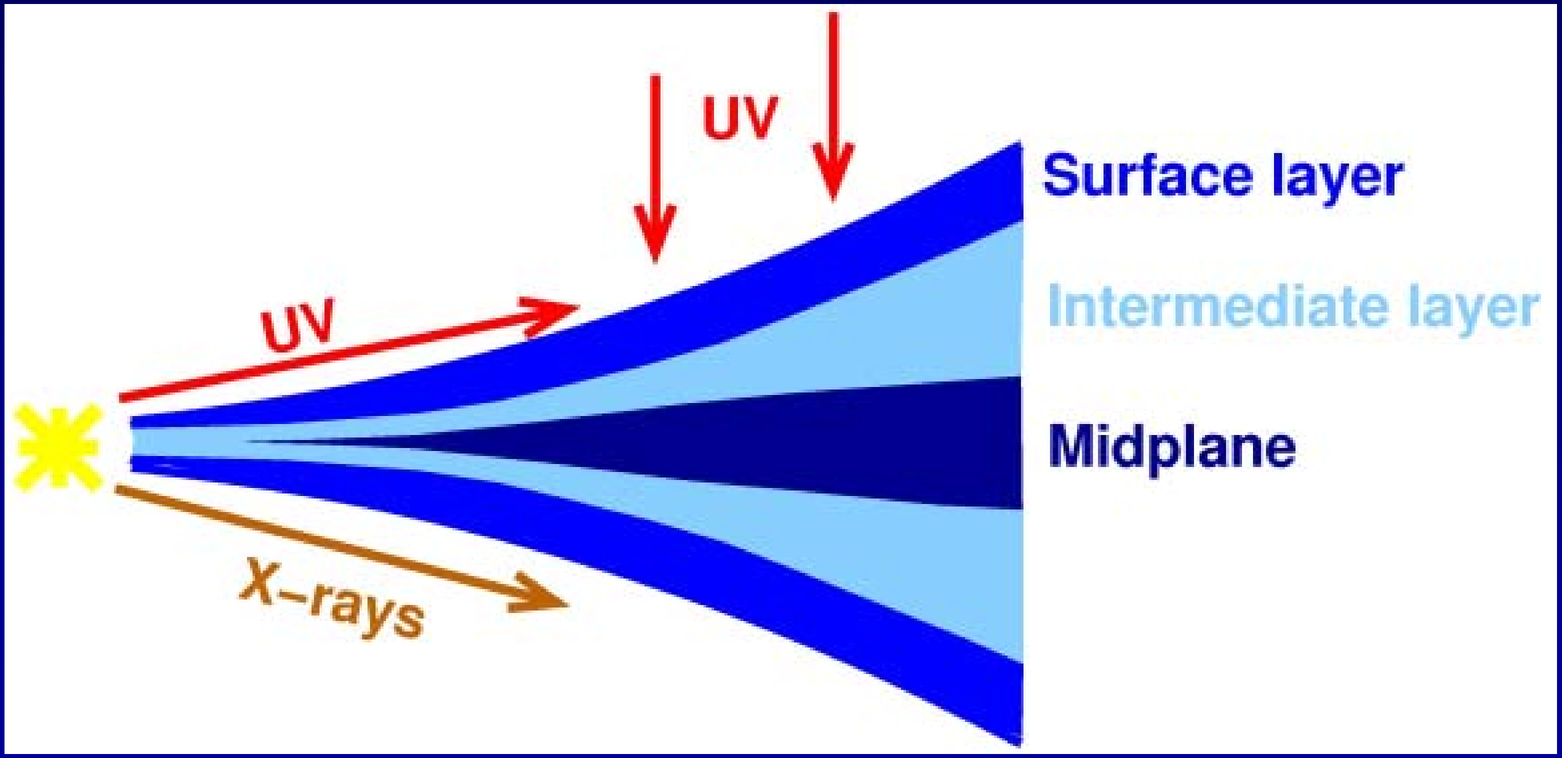
Aikawa et al. 1999

Flaring disk models (>50 AU)

- **Calculate chemistry in vertical and radial directions in 1+1D static flaring models**
  - ***Aikawa et al. 1999, 2001:***
    - **Kyoto minimum solar mass disk model**
    - **Low temperatures => needed artifically low sticking coefficient S=0.03 to match observations**
  - ***Willacy & Langer 2000***
    - **Two-layer Chiang & Goldreich model**
    - **All molecules photodissociated in warm layer**
    - **All molecules frozen on grains in cold layers => needed high photodesorption rate to match observations**
  - ***Aikawa et al. 2002, van Zadelhoff et al. 2003***
    - **D'Alessio et al. models with continuous T,n gradient**
    - **Warm molecular layer where molecules stay off the grains even with S=1**
- **No radial or vertical mixing included, but models allow important processes and parameters to be identified**
  - **Chemo-hydrodynamical models by Markwick et al. 2003, Ilgner et al. 2004 focus on inner 10 AU**

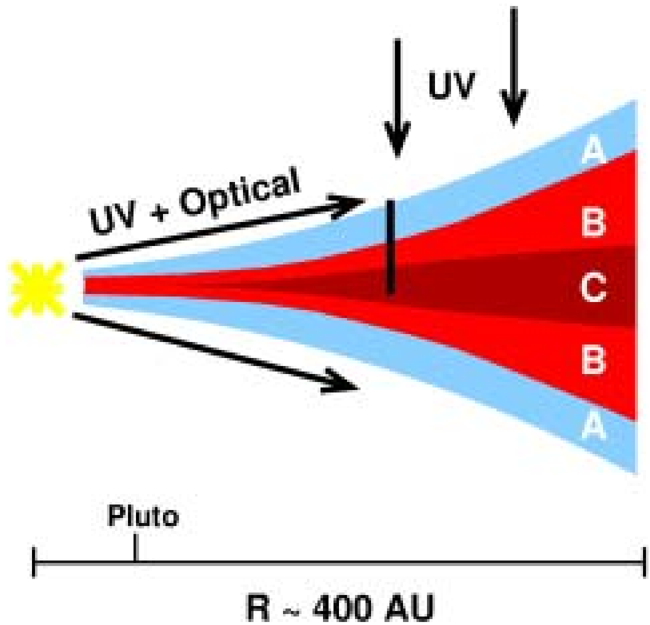
Chemical structure of disks

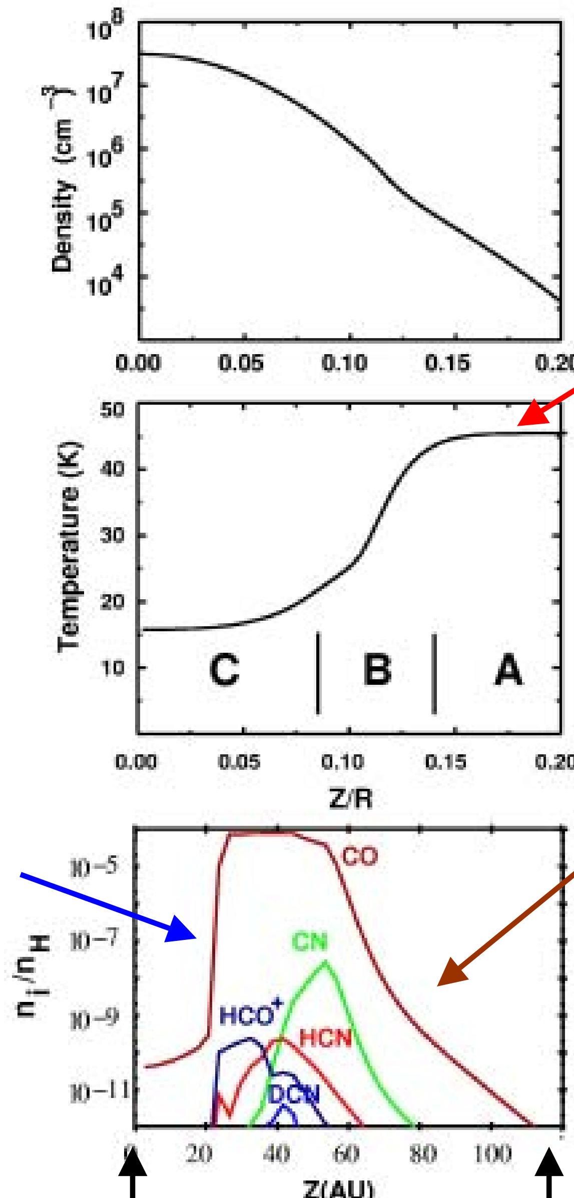
- Surface layer: molecules dissociated by UV photons
- Warm intermediate layer: molecules not much depleted, rich chemistry
- Cold midplane: molecules heavily frozen out



⇒Chemistry dominated by UV in upper layers and by temperature profile in intermediate-midplane layers

Vertical structure (R=200 AU)





T_{gas} is larger

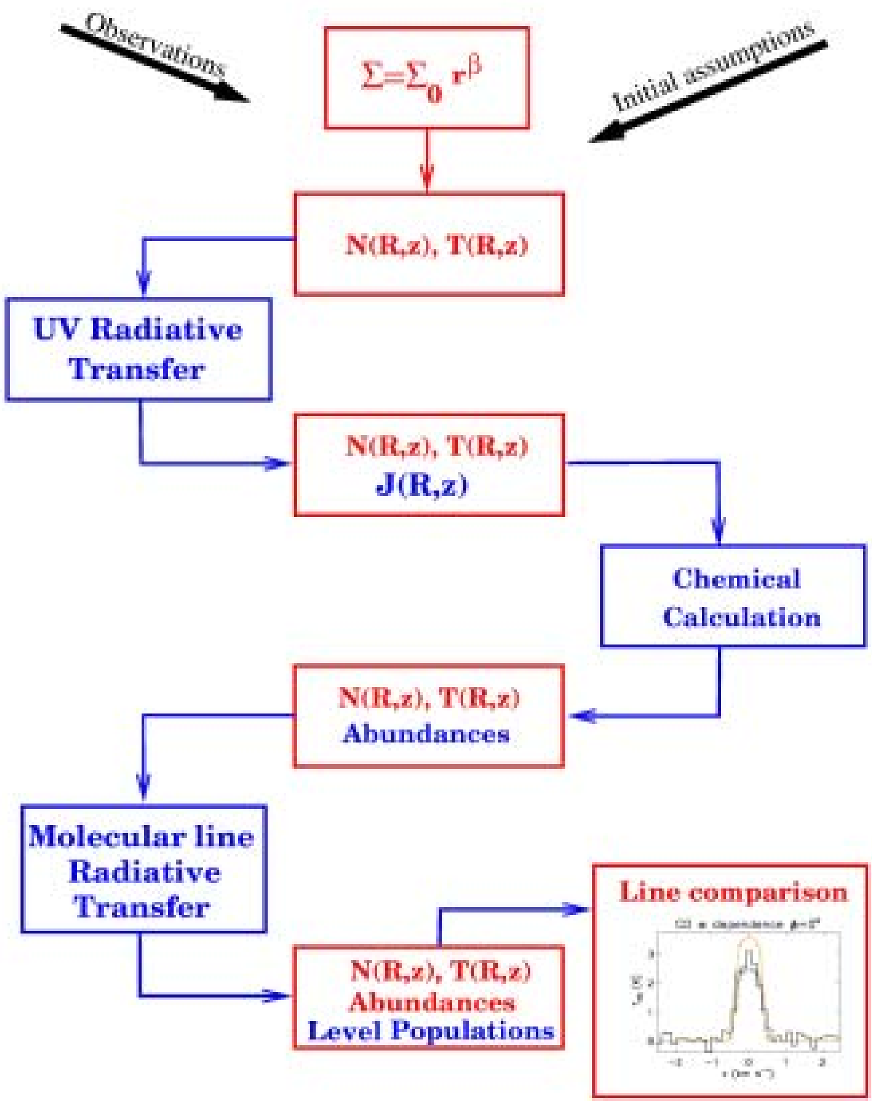
Freeze-out

Photodissociation

midplane

surface

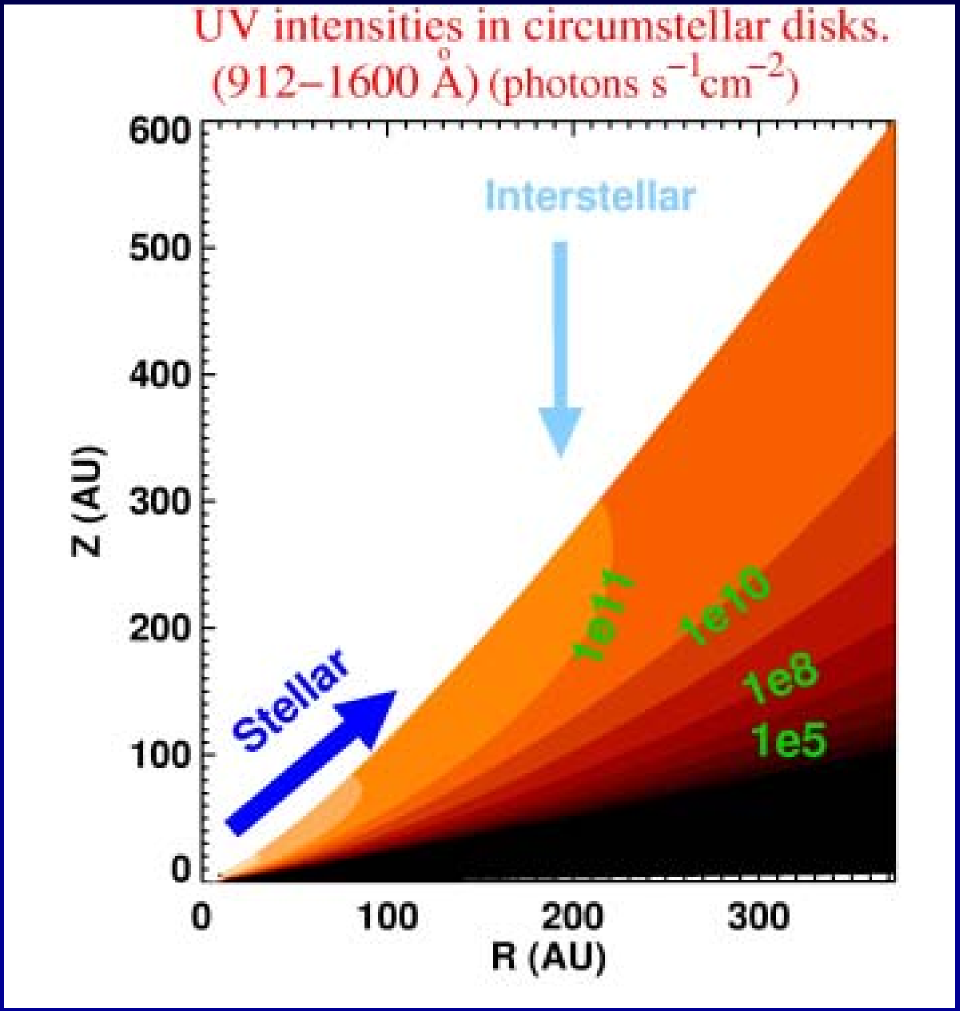
Model flowchart



- Many recent efforts concentrate on calculating T(gas) self-consistently
- T(gas)>>T(dust) in upper layers => outgassing?

Van Zadelhoff et al. 2001
Jonkheid et al. 2004
Kamp & Dullemond 2004
Hollenbach & Gorti 2004

Importance of shape and treatment UV radiation field



Full 2D calculation including absorption and scattering

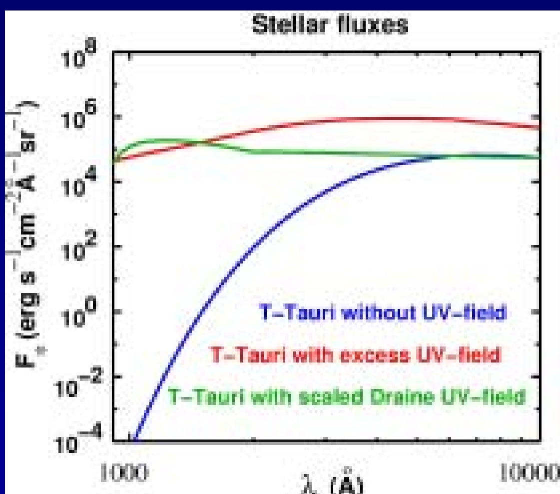
Penetration depth depends on optical properties grains

Van Zadelhoff et al. 2003

Normal ISRF: ~1x10^8 ph s^{-1} cm^{-2}

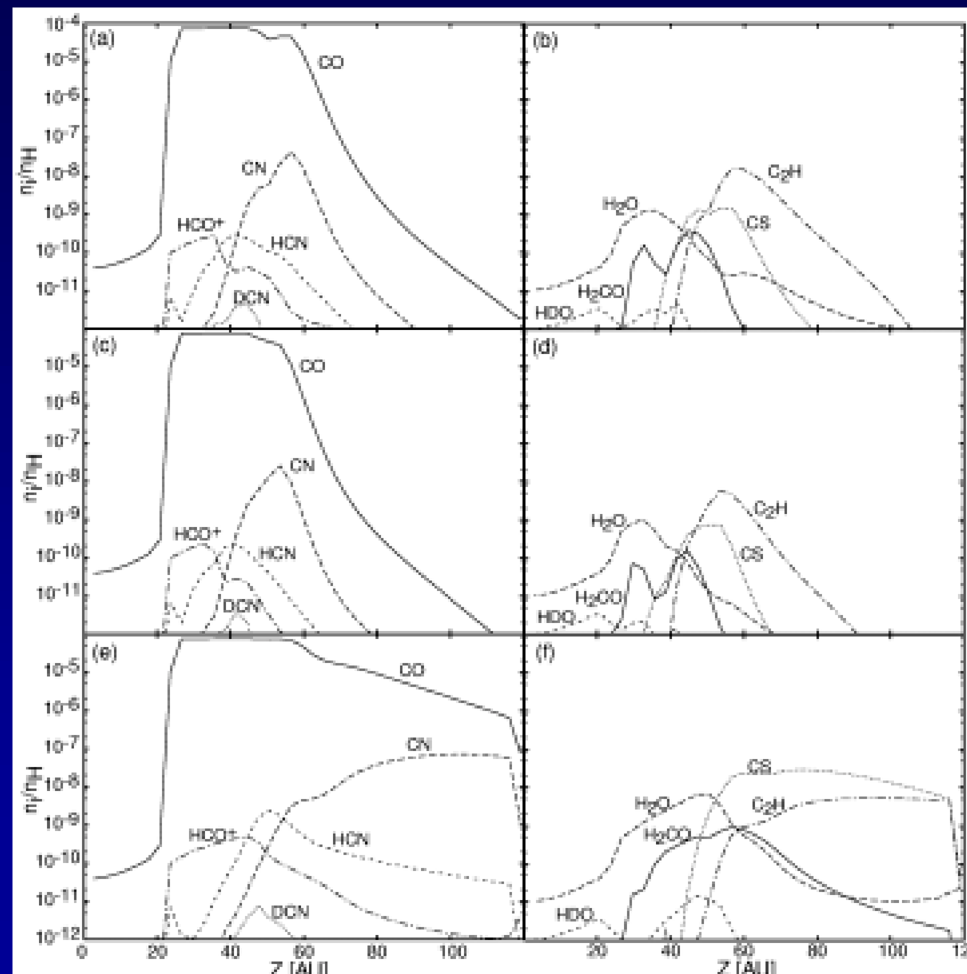
⇒Enhanced by factor > 1000 in upper layers

Effect of stellar far-UV



Midplane

Surface



Green

Red

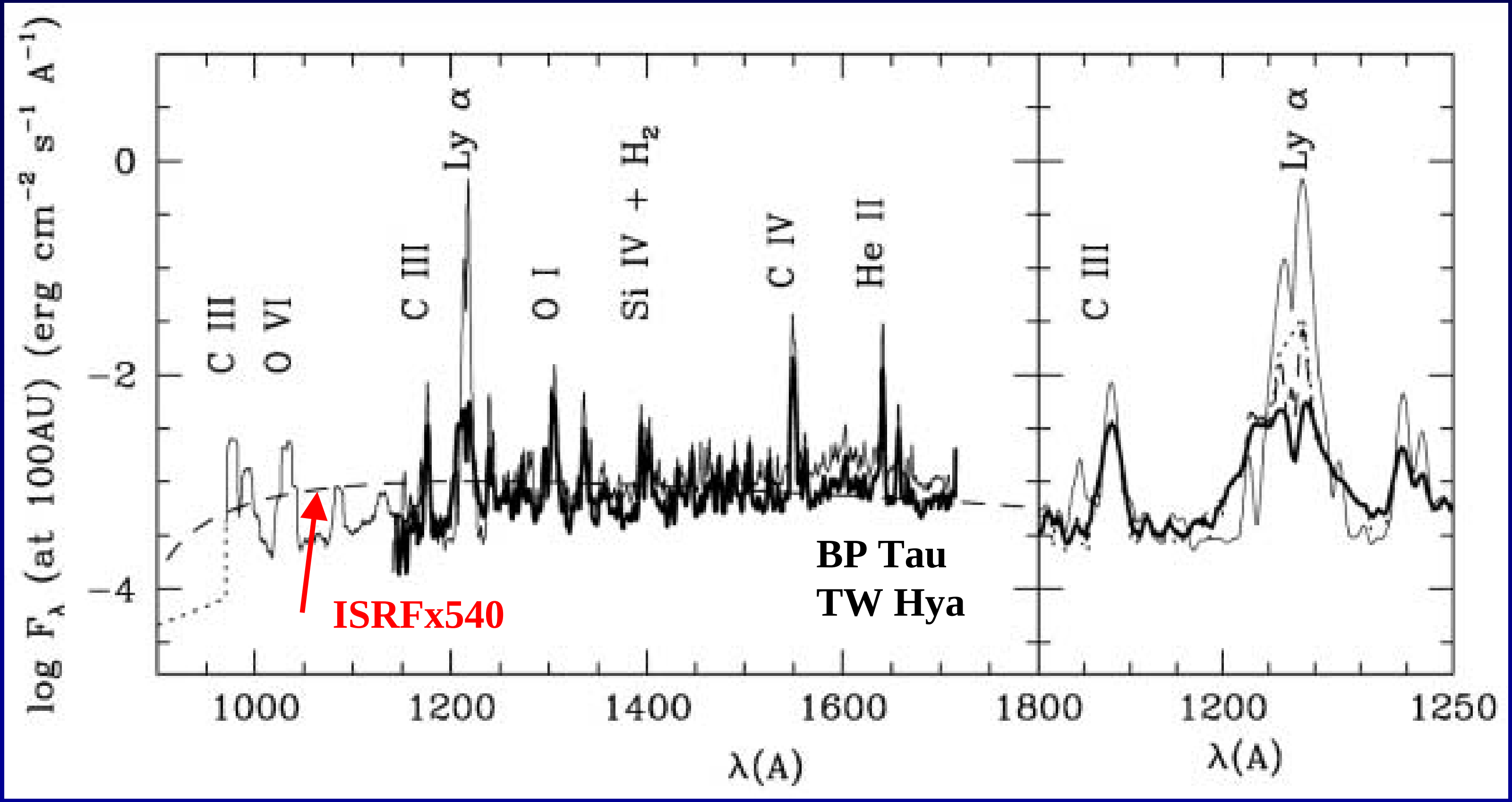
Blue

=> Molecules extended to greater height if no far-UV

Van Zadelhoff et al. 2003

Importance of Lyman α

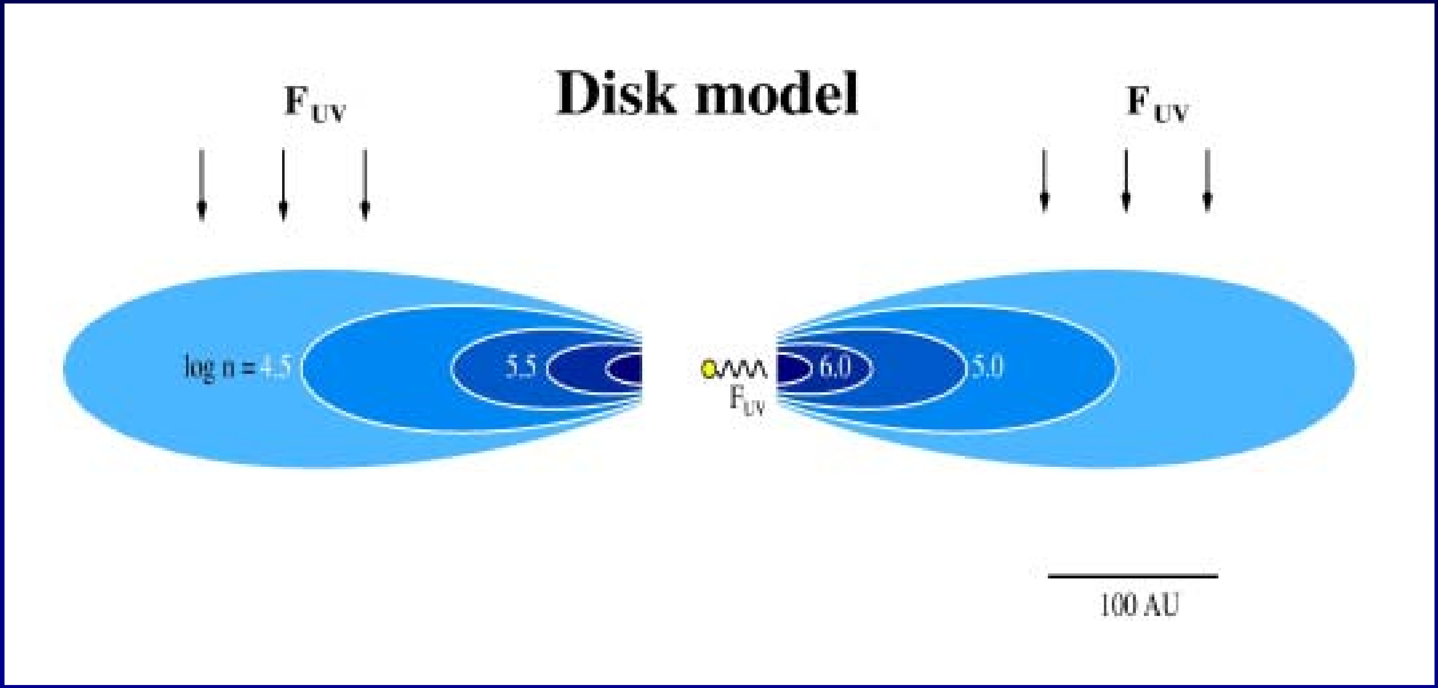
Observed FUV spectra of T Tauri stars



- Photodissociation rate $k_{pd} = \int \sigma(\lambda) I(\lambda) d\lambda$
- Some molecules are dissociated by Lyα (e.g., H_2O, HCN), others are not (e.g. CN, CO, H_2)

Bergin et al. 2003

Models: tenuous 'transitional' disks



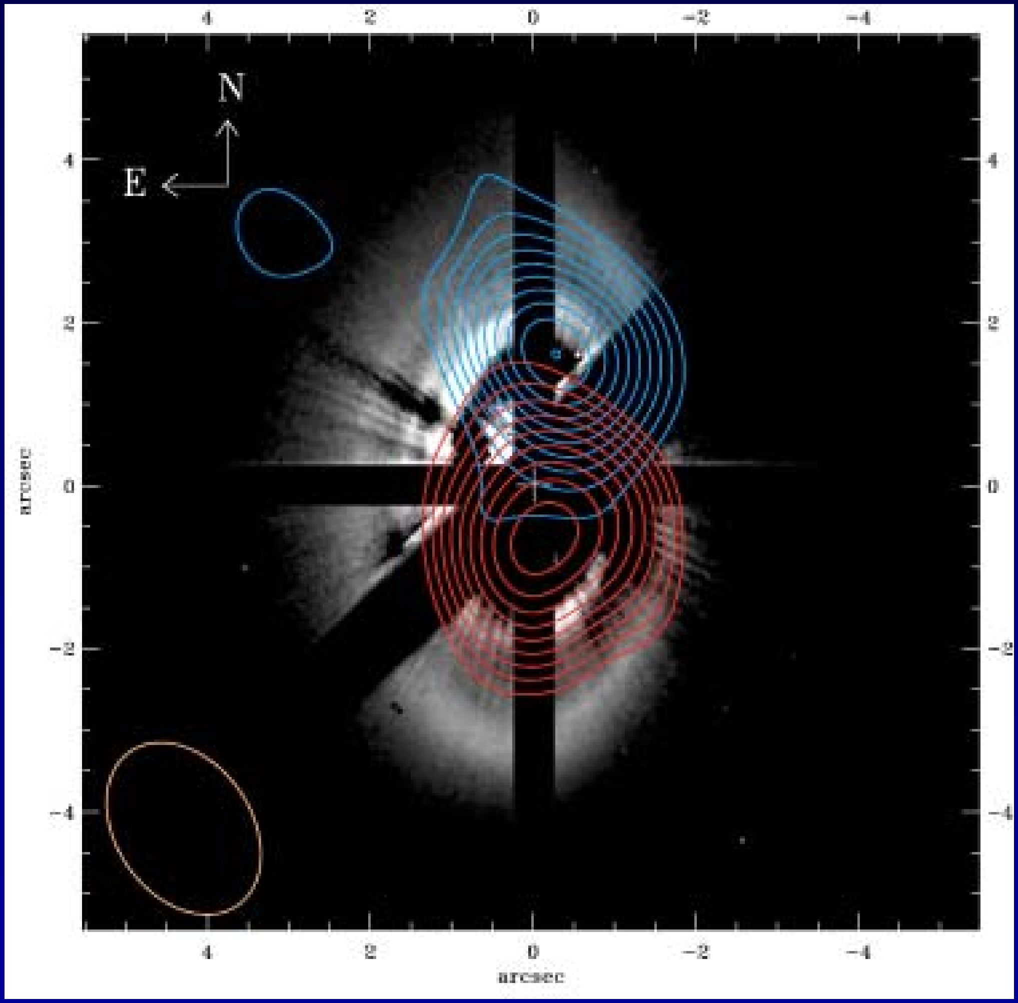
- Disks are optically thin to UV and IR radiation => analytic solution T_{dust}
- Disk masses (gas + dust) of order M_{Earth}, 1000 x less than young disks
- Initial work: A-stars; use stellar atmosphere model for stellar radiation
- Recent work: extension to G-stars including chromosphere

Kamp & Bertoldi 2000, Kamp & Samnar 2004

HD 141569 transitional disk: dust and cold gas

Massive gas-rich disk

Debris disk



IRAM PdB

^{12}CO 2-1

Superposed on HST-STIS

When does gas disappear from disk? => constraints on time scale giant planet formation

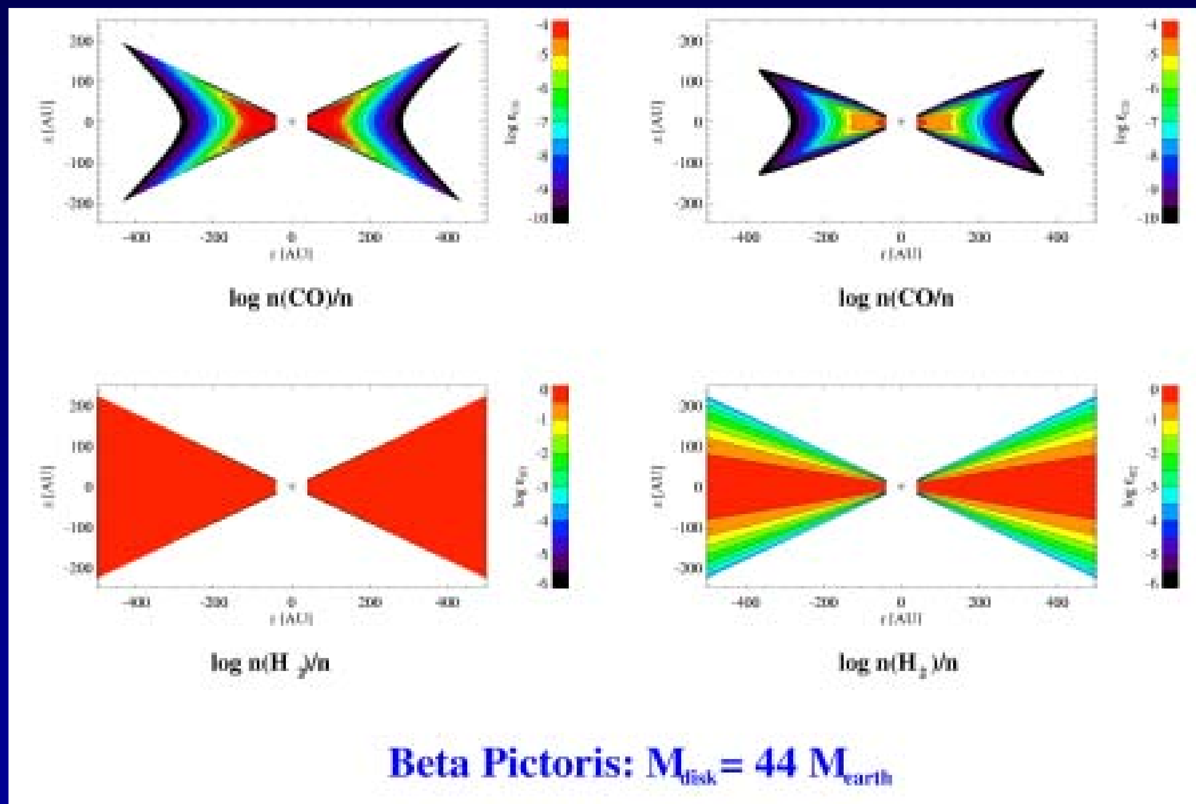
Augereau, Dutrey et al. 2004, in prep

CO vs H_2

Stellar UV | Stellar + interstellar UV

CO

H_2



CO p.d. + Frozen out

H_2 self-shielding

=> Absence of CO does not mean absence of H_2!

Note: both CO and H_2 are only dissociated at 912-1100 Å

Kamp & Bertoldi 2000

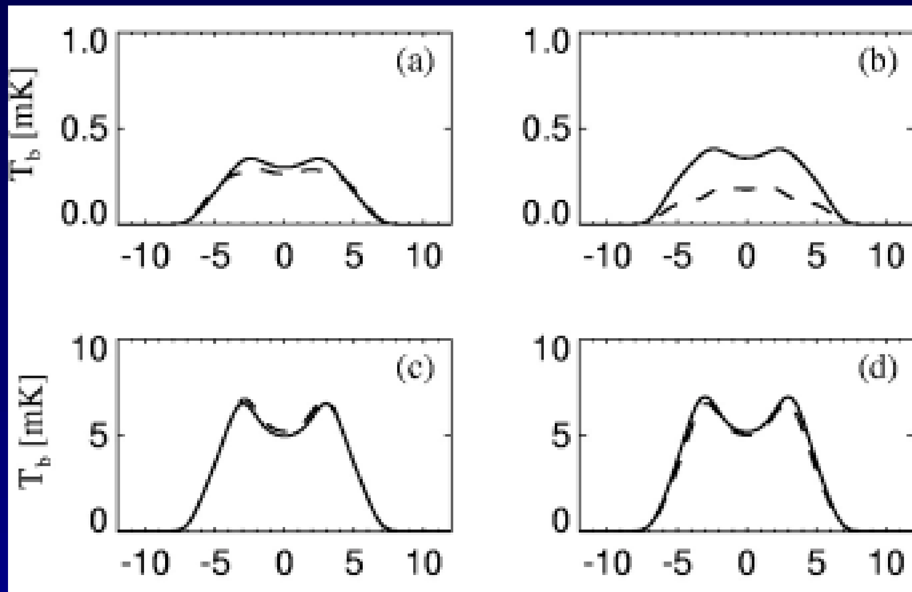
C and C^+ as gas tracers of tenuous disks

V_{drift}=max V_{drift}=0

βPic

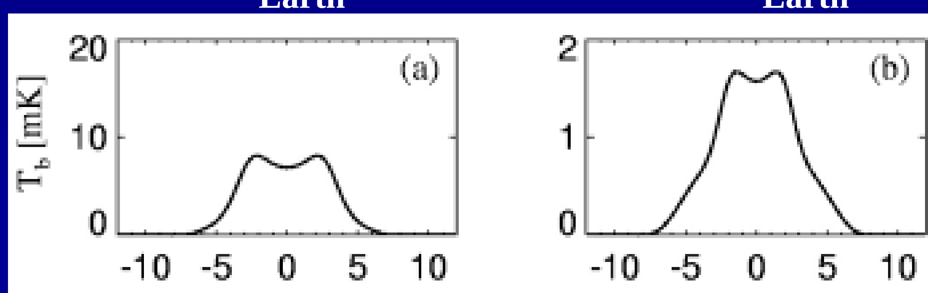
0.2 M_{Earth}

2 M_{Earth}



[C I]

2 M_{Earth} 0.2 M_{Earth}



[C II]

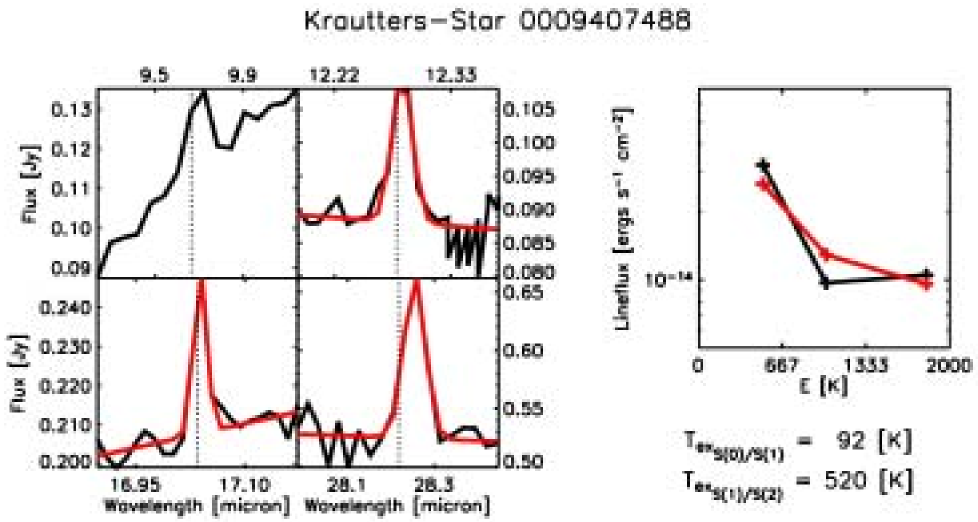
- Lines should be detectable by future facilities (APEX, SOFIA, Herschel)
- Mid-IR lines (e.g. [S I] 25 μm) alternative tracers

Kamp et al. 2003
Gorti & Hollenbach 2004

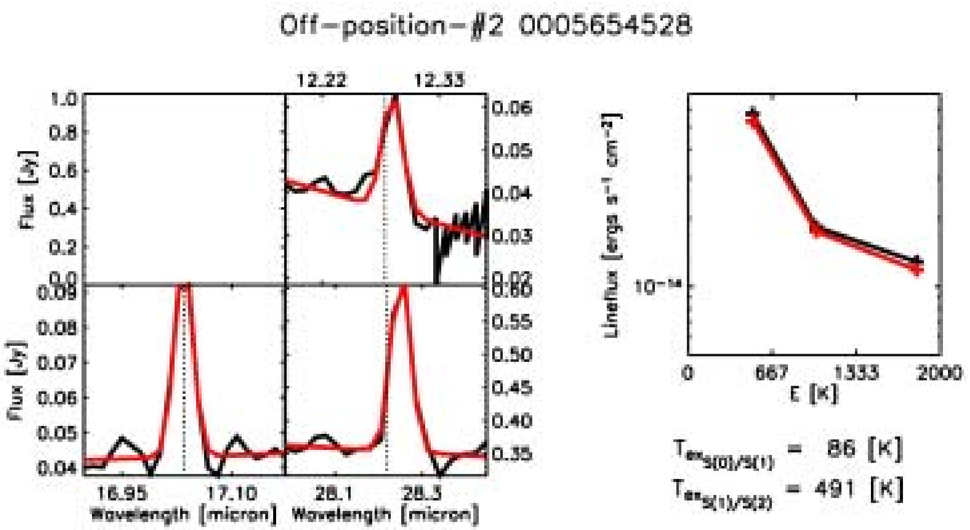
Conclusions

- Gas-phase and solid-state species are starting to be observed in outer regions of disks
- Most observed emission and chemistry comes from warm intermediate layer where photoprocesses and thermal desorption play a role
- Significant freeze-out in cold midplane (>20 AU)
- Gas-phase and solid-state bands are useful probes of density and temperature structure
- CO is not a good tracer of gas mass => need to consider alternatives (H_2, C, C^+, …)
  - Need high spectral resolution to get sufficient line/continuum ratio
- Current view hampered by lack of spatial resolution and sensitivity
  - Future mm/IR facilities, i.p. ALMA, JWST-MIRI, ELT, IR interferometry
  - Unique contributions TPF/Darwin will depend on its spectroscopic capabilities

H_2 lines with Spitzer



Krautter's star



Random off position

H_2 lines detected on source, but also at off positions

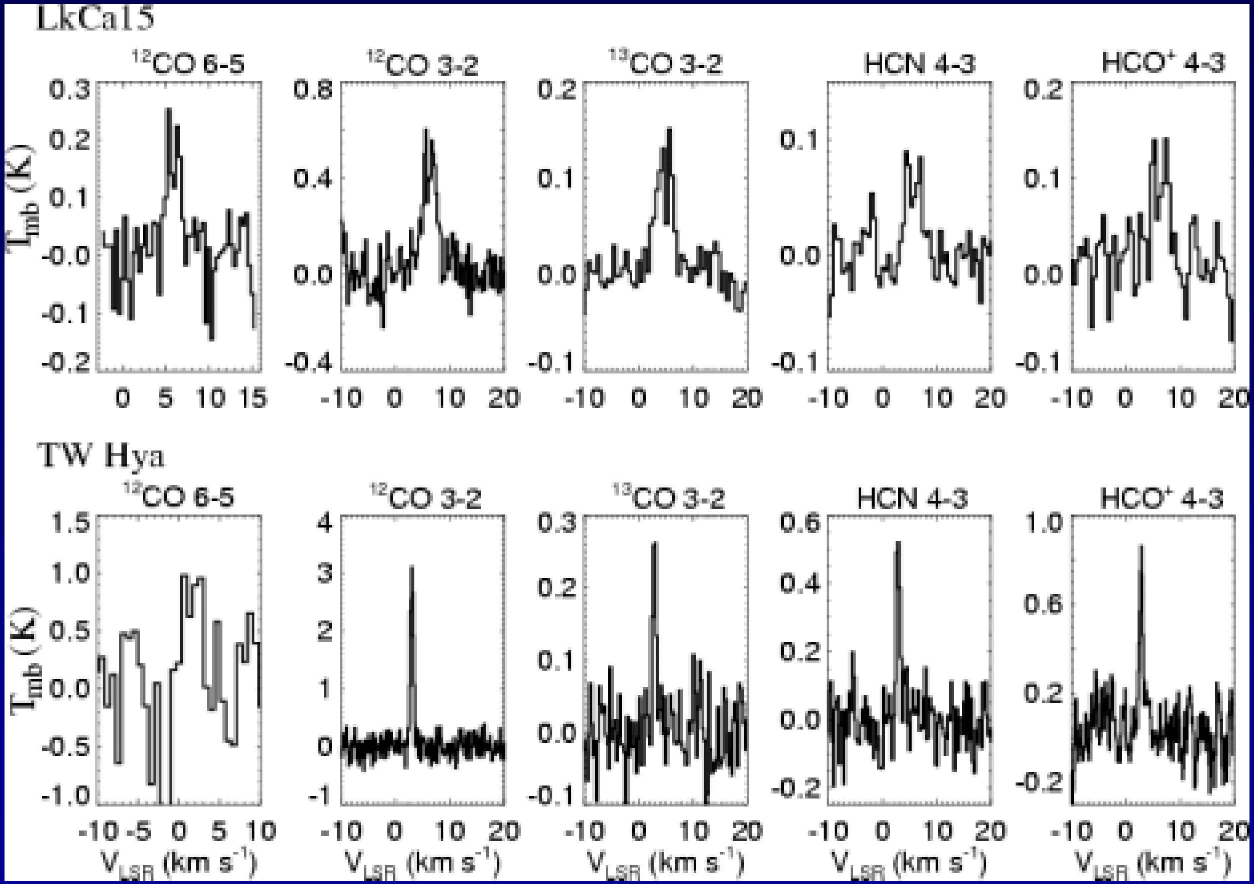
Observational gas tracers

- CO mm:
  - detected in some cases but not good mass tracer (photodissociation, freeze-out)
- H_2 pure rotational lines:
  - Pro: main reservoir of gas, does not freeze-out, lines optically thin
  - Con: difficult to observe (low line/cont), only probes warm (>80 K) gas
- H_2 and CO IR/UV lines:
  - detected in several cases, but arise mostly from small amount of high-T gas in inner region
- [C I], [C II], [O I], [S I] fine-structure lines:
  - Results somewhat model dependent

Summary chemistry

- **Does chemistry affect disk structure?**
  - **Gas temperature in upper disk layers can be significantly higher than that of dust (see talks tomorrow) => affects vertical structure and line emission; chemistry determines abundances coolants O, C^+, C and CO**
  - **Freeze-out and dust destruction modify grain opacities**
  - **Ionization fraction => affects magnetohydrodynamics (but can probably be estimated by small network)**

Submillimeter lines



First detection CO 6-5 emission from disk using CSO

Van Zadelhoff et al. 2001

Some observational findings

- **Simple gas-phase molecules observed**
  - **Ion-molecule reactions (HCO^+)**
  - **Photon processes (high CN/HCN)**
  - **High deuterium fractionation (DCO^+)**
  - **Low abundances complex species (H_2CO, CH_3OH)**
- **Data only sensitive to >50 AU**
- **Lines comes from warm 20-40 K layer with $n=10^6$-10^8 cm^{-3}**
- **Disk-averaged abundances are "depleted" by factor of 5-100 (using mass from dust continuum and assuming gas/dust=100)**
- **Solid CO and H_2O detected in edge-on disks**

Summary chemistry

- **Inner disks: highly sophisticated models including radial transport and vertical mixing being developed, but no observational tests yet (need full ALMA with 64x12m)**
- **Outer disks: 1+1D static flaring disk models reproduce submillimeter lines of simple species within factors of few**
  - **Emission comes from intermediate warm layer**
  - **Chemistry in warm layer dominated by photodissociation and thermal desorption => important to know T_{dust} and UV field accurately**
  - **Molecules strongly depleted in cold midplane => high deuteration fraction**
  - **CO is not a good gas mass tracer (alternatives H_2, C, C^+ to be determined)**
  - **Importance of vertical mixing to be determined: can chemistry put limits?**

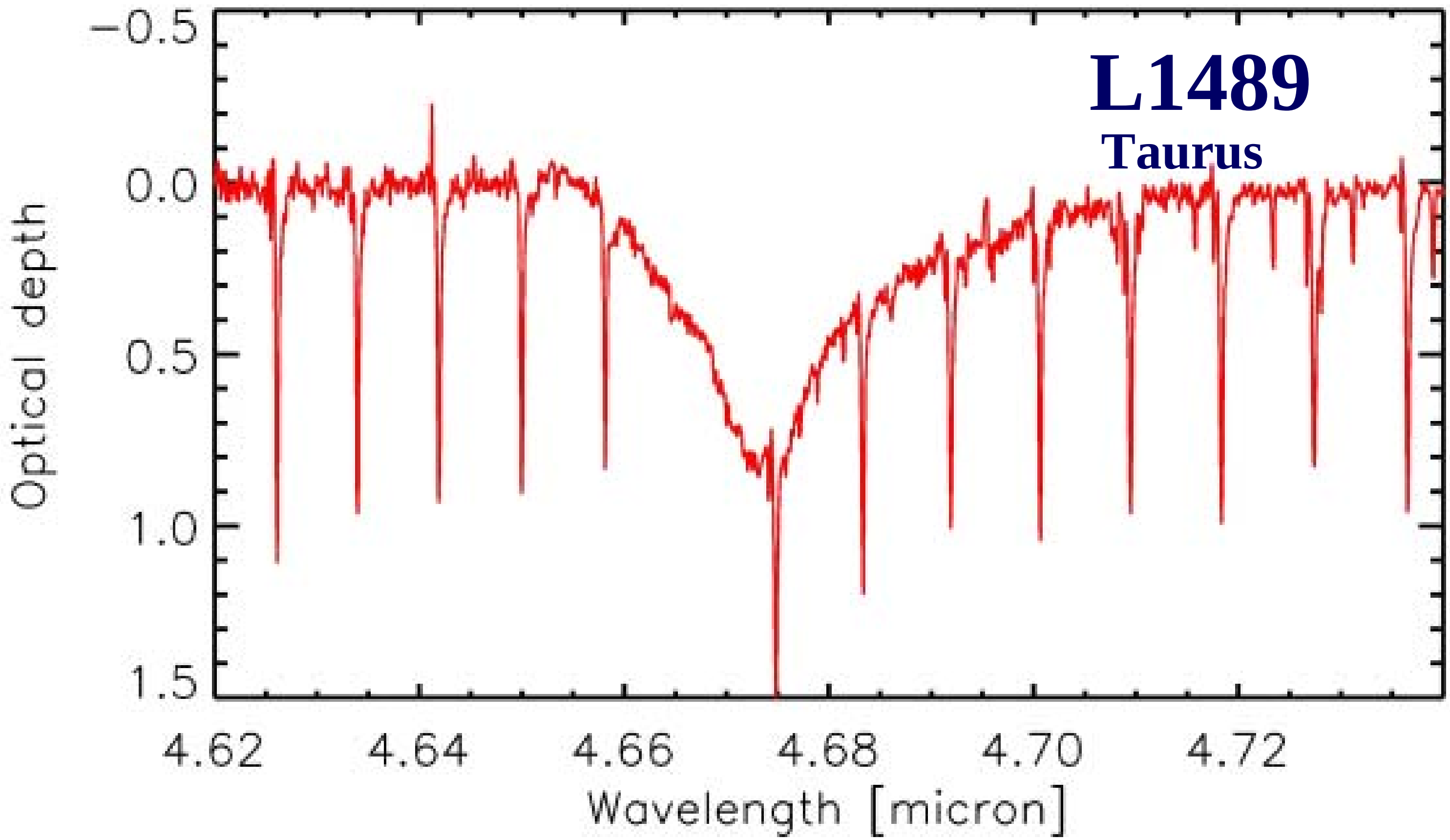
Molecular abundance ratios

Type	Object	HCO^+/CO	CN/HCN
T Tau	LkCa 15	1.6(-5)	7.9
	TW Hya	5.0(-5)	7.1
	DM Tau	2.8(-5)	5.1
Herbig Ae	HD 163296	2.7(-5)	>12.4
	MWC 480	1.5(-5)	>11.7
Protostar	IRAS16293	1.8(-5)	0.05
Dark cloud	TMC-1	1.0(-4)	1.5
PDRs	Orion Bar	2.0(-5)	3.8
	IC 63	2.7(-5)	0.7

D/H ratios

Object	Molecule	D/H
Hot cores	DCN/HCN	0.005-0.02
Dark cloud	DCN/HCN	0.023
	DCO^+/HCO^+	0.015
Low-mass	DCN/HCN	0.013
protostar	DCO^+/HCO^+	0.086
Disk (TW Hya)	DCO^+/HCO^+	0.035
Comet	DCN/HCN	0.002 nucleus
		0.09 jet
	HDO/H_2O	0.00032

Solid and gaseous CO toward a young, large edge-on disk



Keck
R=25,000

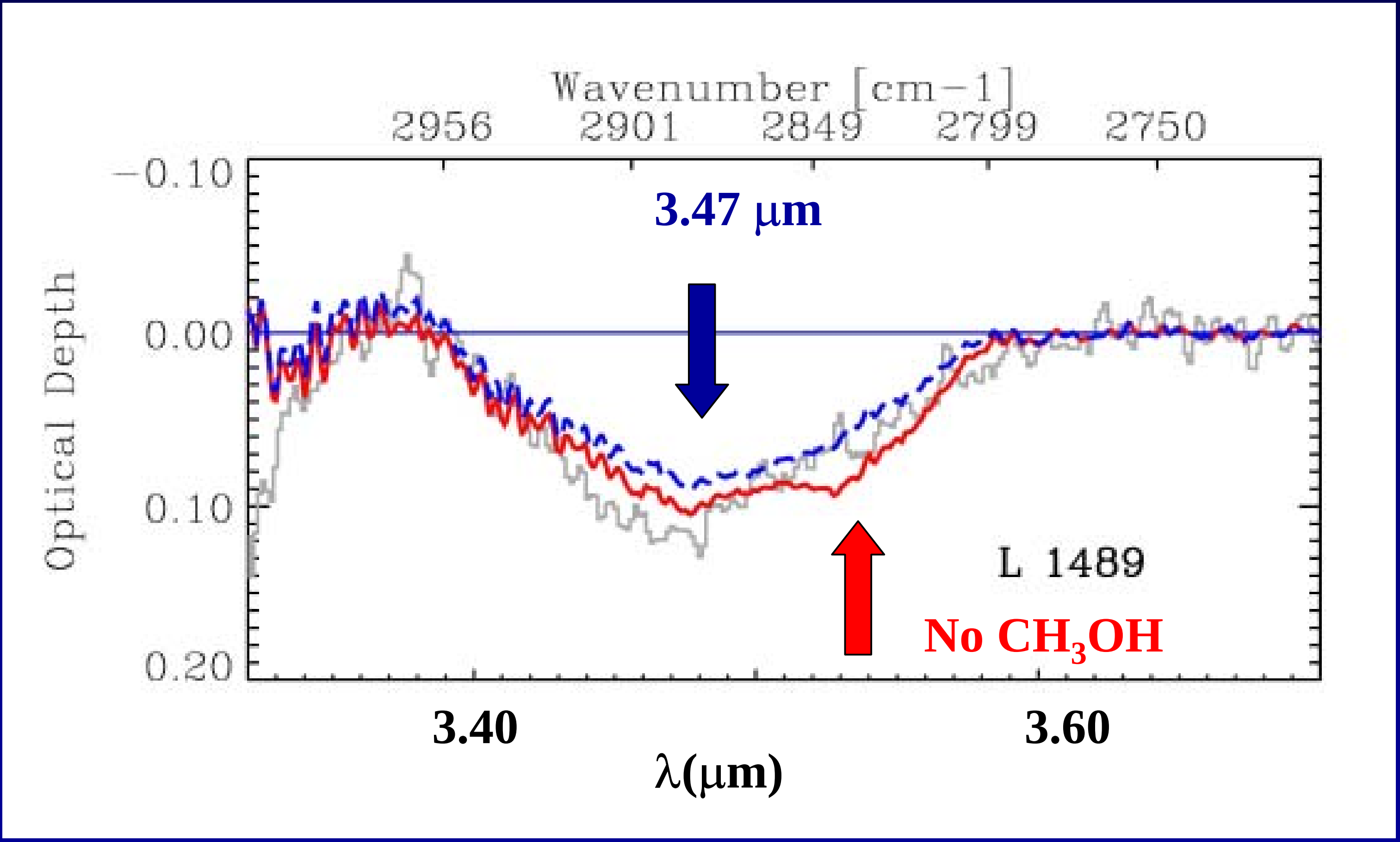
- **Red wing line profiles traces accretion to within 0.1 AU from star**
- **Warm CO gas (up to 200 K), with CO_{gas}/CO_{solid}~10**

See also: Shuping et al. 2001

Boogert, Hogerheijde & Blake 2002

Search for solid methanol

Key ingredient for building complex organic molecules

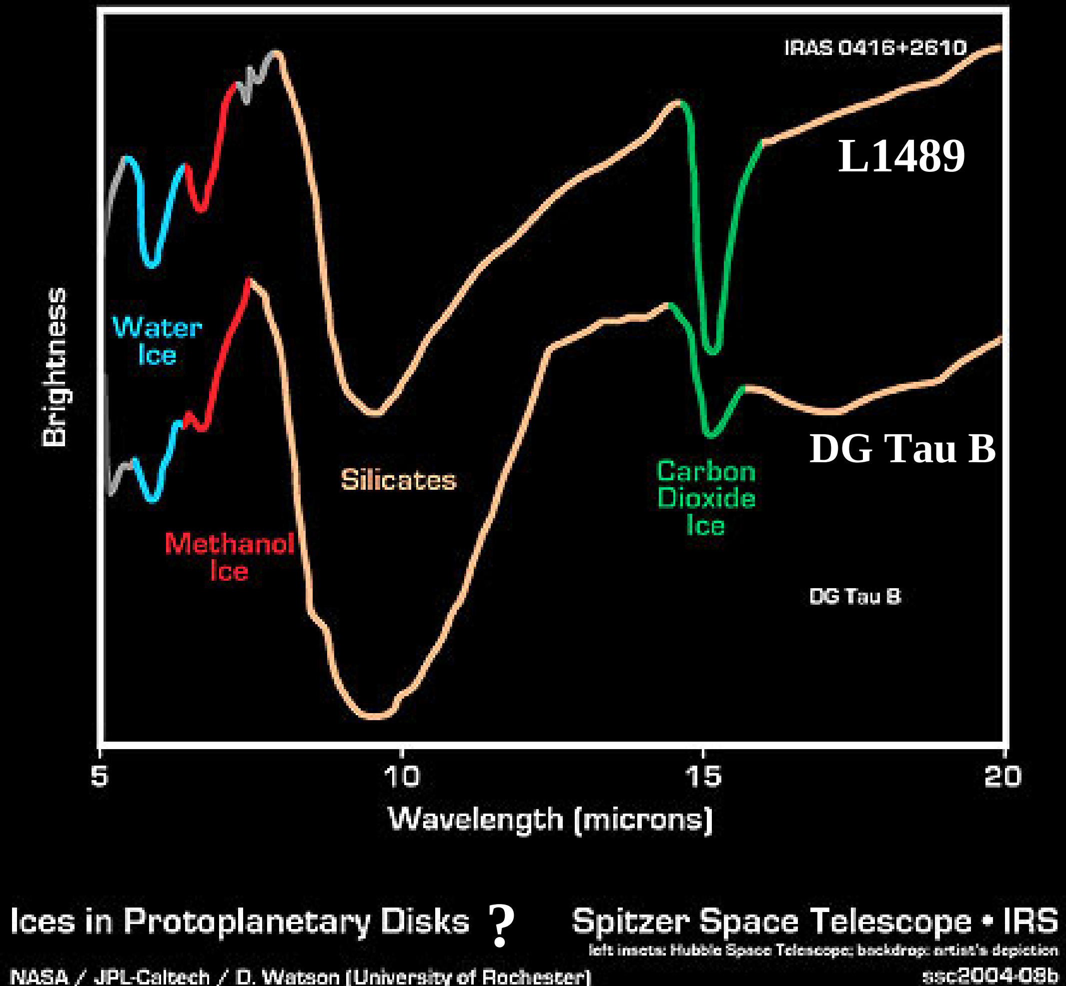


3.47 μm feature, but no 3.54 μm CH_3OH

=> CH_3OH/H_2O < 5% in L1489 disk

Pontoppidan et al. 2003

Spitzer observations of edge-on disks

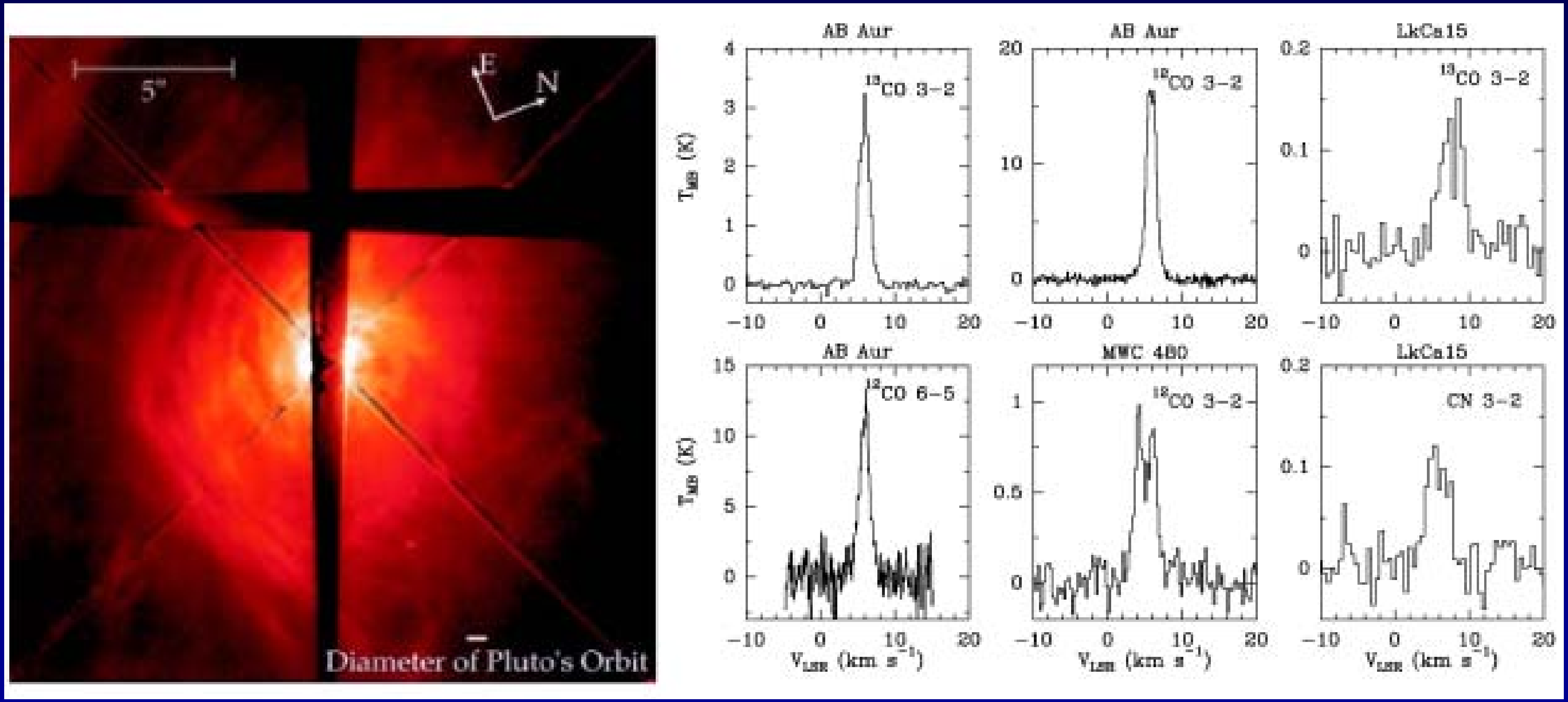


- Ices may arise primarily in outer envelope

Watson et al. 2004

Example: AB Aur

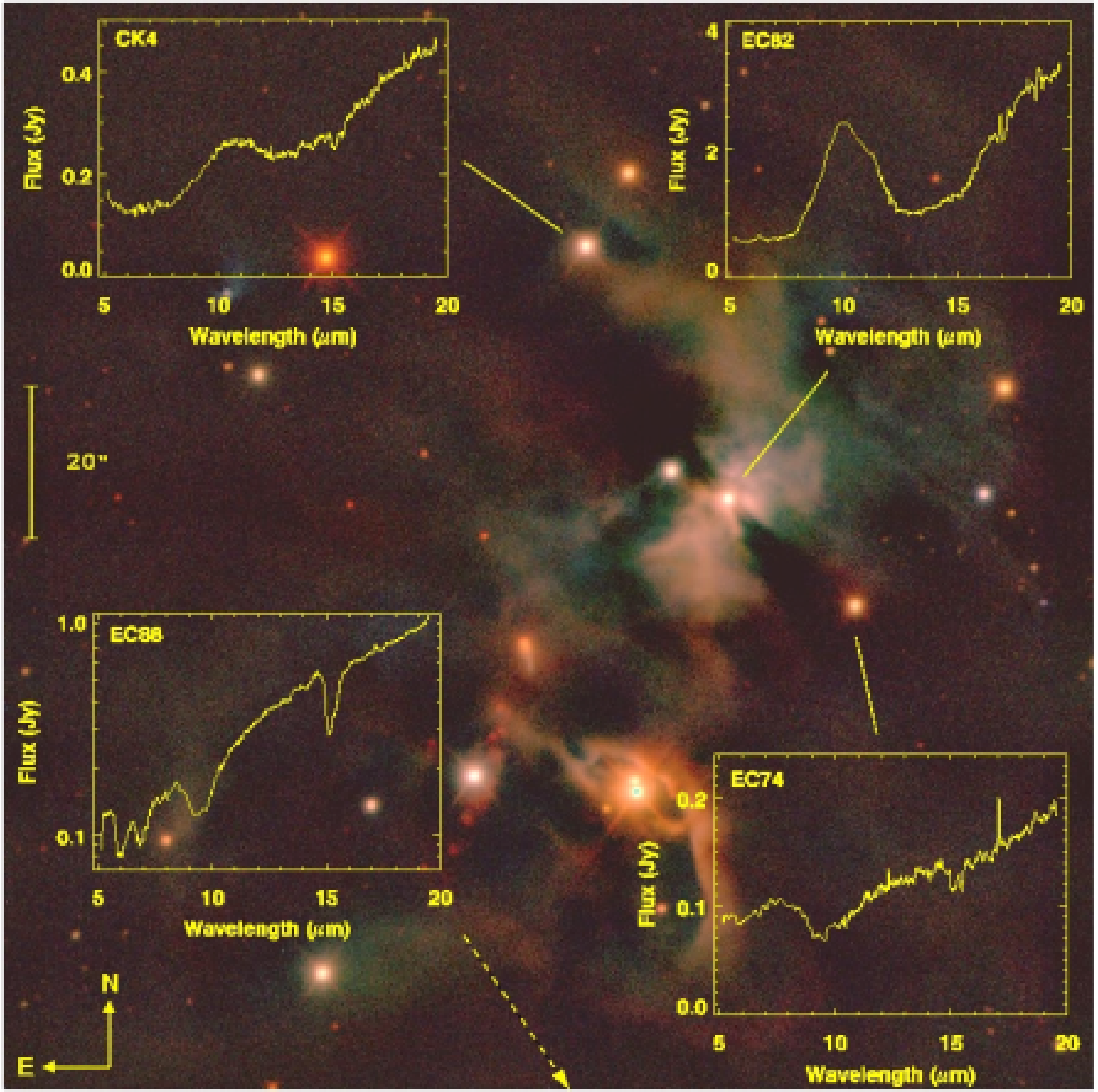
Emission dominated by extended envelope



Note strong CO 3-2 and 6-5 lines!

Van Zadelhoff et al. 2001
Bacmann, Schreyer et al. in prep.

Spitzer spectra of low-mass YSO's
Serpens core

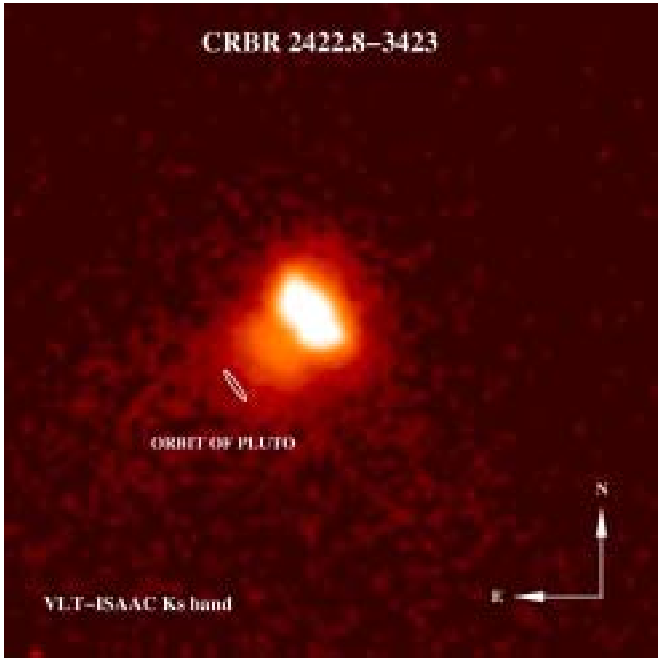


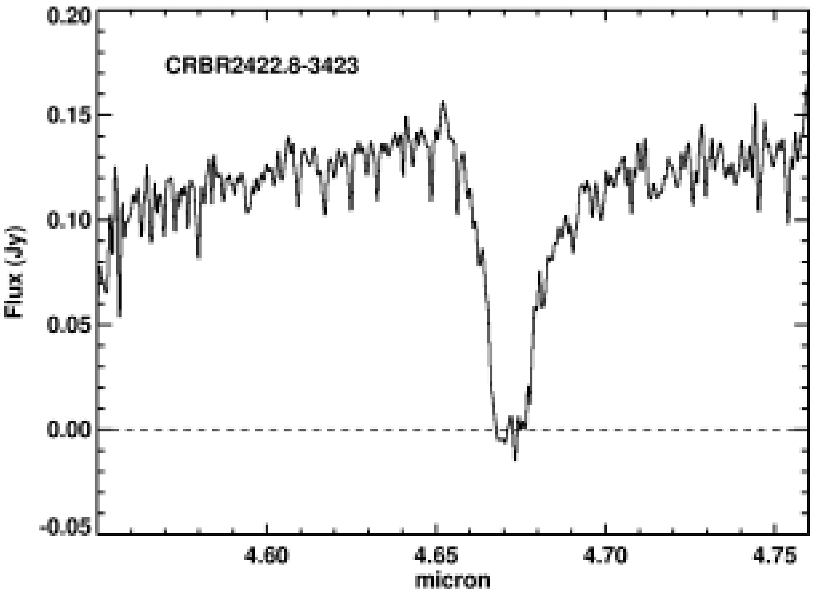
VLT-ISAAC
J, H K image

c2d team data

Detection of abundant solid CO in an edge-on circumstellar disk

VLT-ISAAC





VLT-ISAAC K'

Brandner et al. 2000

CO_{gas}/CO_{solid} ~1

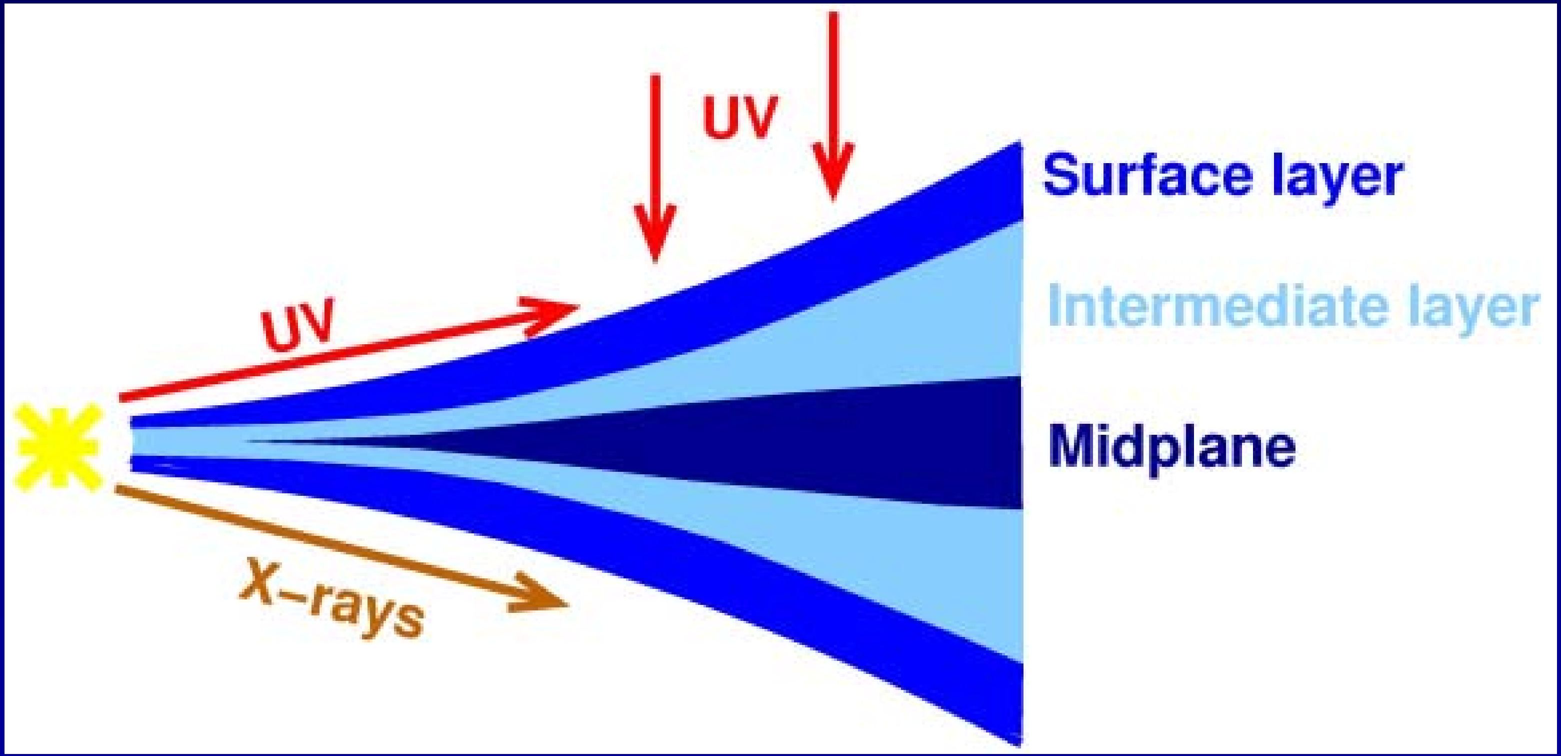
$T_{ex}(CO)$~50 K

Contamination by foreground cloud estimated to be small

Thi, Pontoppidan, vD et al. 2002

Chemical structure of disks

- Surface layer: molecules dissociated by UV photons
- Warm intermediate layer: molecules not much depleted, rich chemistry
- Cold midplane: molecules heavily frozen out



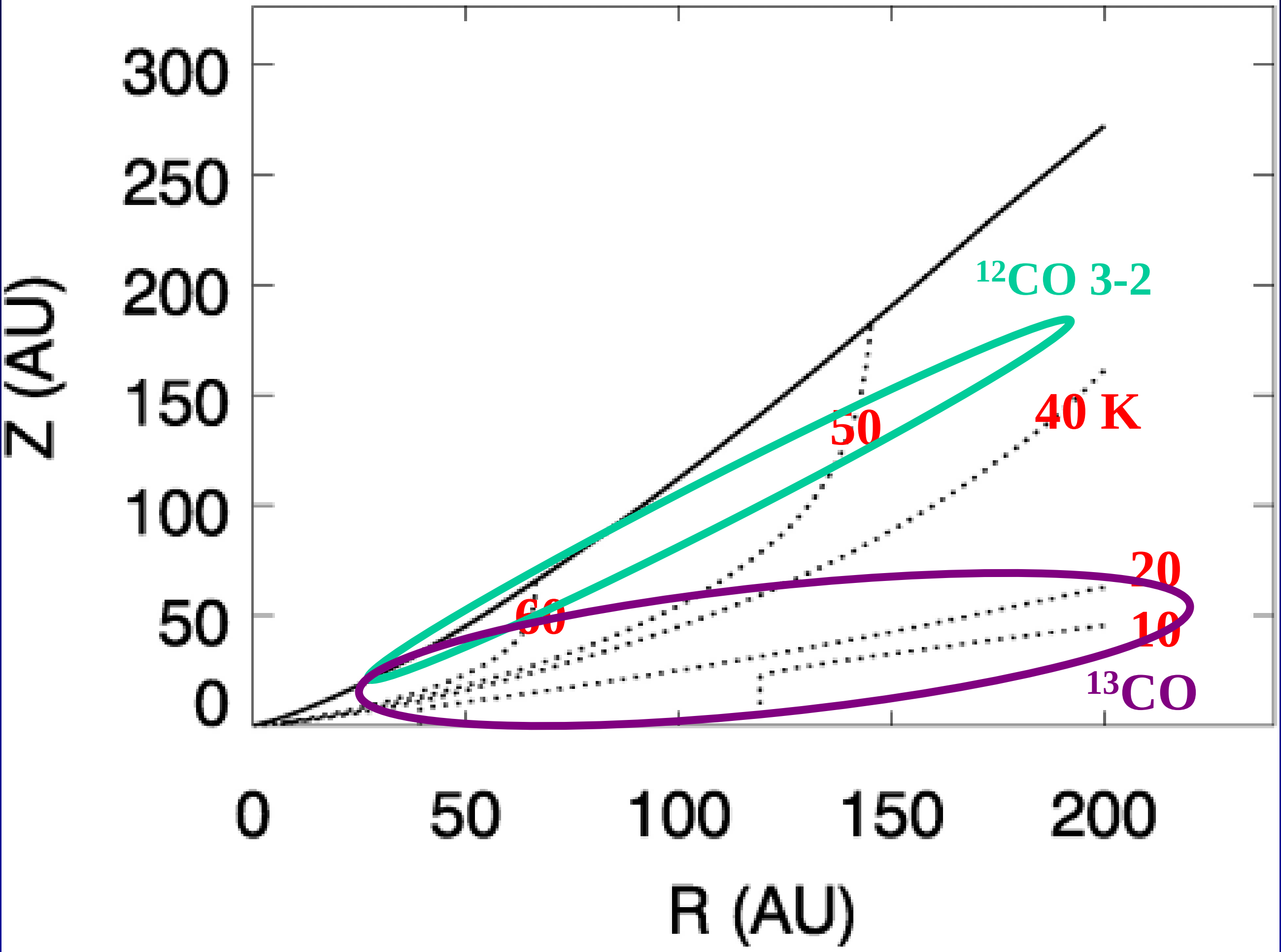
Aikawa & Herbst 1999
Aikawa et al. 2002

Willacy & Langer 2000
Van Zadelhoff et al. 2003
Markwick et al. 2002
Ilgner, Henning et al. 2002

Summary chemistry

- Submillimeter lines of simple species observed, e.g. HCO^+, H_2CO, HCN, CN
- Emission comes from intermediate warm layer
- Chemistry in warm layer dominated by photodissociation and thermal desorption
- Molecules strongly depleted in cold midplane

Temperature structure



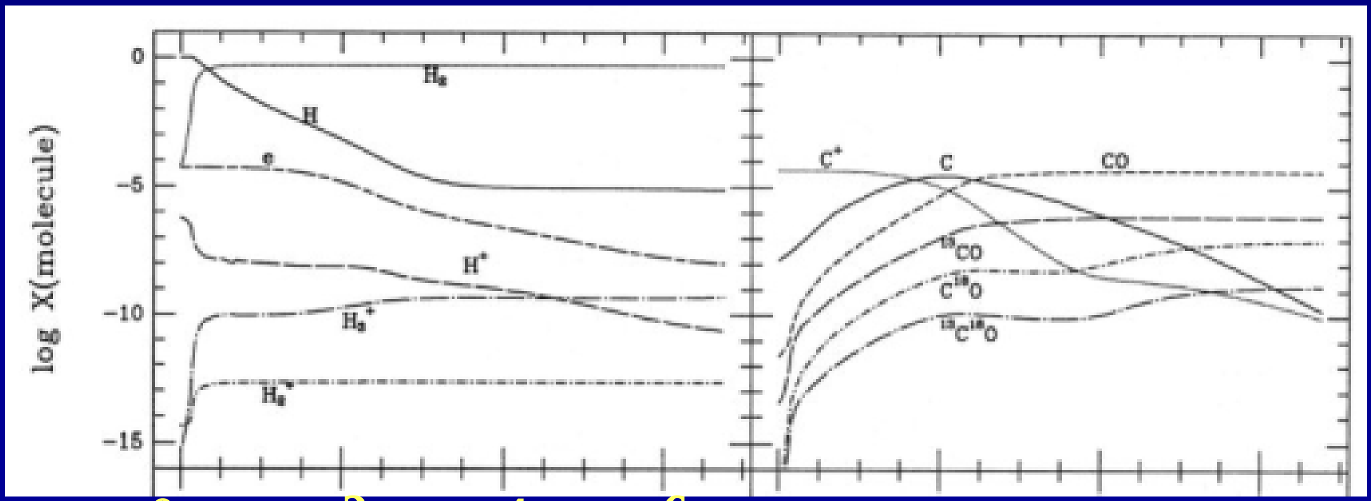
- ^{12}CO τ=1 surface near top of disk
- ^{13}CO emission from entire disk

Van Zadelhoff et al. 2001
Dartois et al. 2003

A few words about chemistry

Gas-phase chemistry

- **Chemistry in upper layers resembles that of a PDR**
  - **Photodissociation H_2 and CO only at 912-1100 Å**
  - **Important to treat H $\rightarrow H_2$ and $C^+ \rightarrow C \rightarrow CO$ transitions accurately (Leiden PDR benchmark workshop), e.g., sensitivities to self-shielding, mutual shielding, PAH abundance, …**
  - **Photorates are rapid => chemical equilbrium in ~10^3 yr**
  - **High abundances of radicals (CN, C_2H, …) in PDR zone**



0 2 4 6

A_V

A few words about chemistry

Gas-phase chemistry

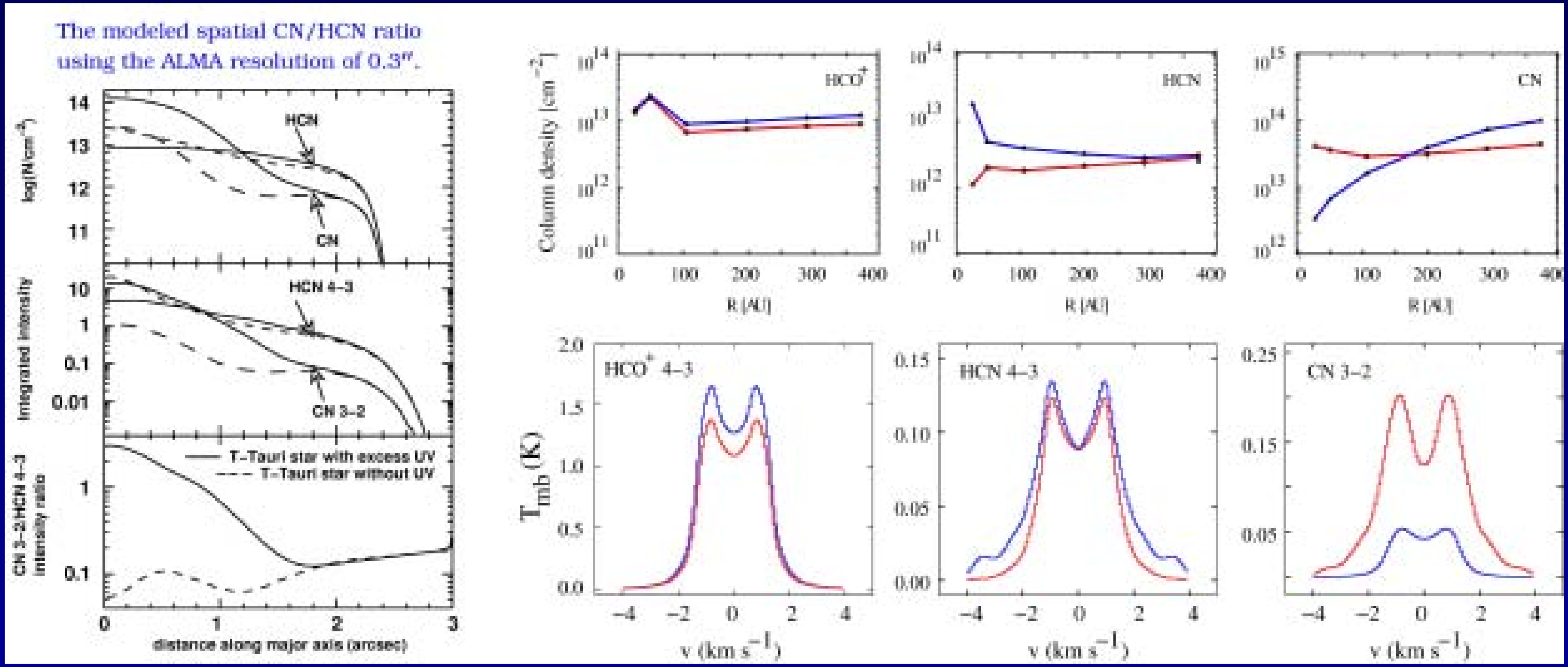
- Elemental abundances (e.g. high vs. low metals) and cosmic ray ionization rate important input parameters
- Gas-phase chemistry not very sensitive to temperature in 10-200 K regime
- Many different chemical networks containing a few hundred to a few thousand reactions => reduction?
  - Wiebe, Semenov et al. 2003, 2004
- Best agreement with well-studied PDRs and dark clouds is a factor of a few – ten => better agreement for disks would be a miracle!

A few words about chemistry

Gas-grain interactions

- Freeze-out/thermal desorption depend sensitively on dust temperature profile
  - Species dependent: CO T>20 K, H_2O T>100 K; binding energies not well known for all species and depend on type of ice or surface
- Fundamental issues with formulation grain surface reactions (diffusion-limited vs. accretion-limited)
- Timescales: $t_{ads} \sim 2 \times 10^9 / n_H$ yr => strongly dependent on density

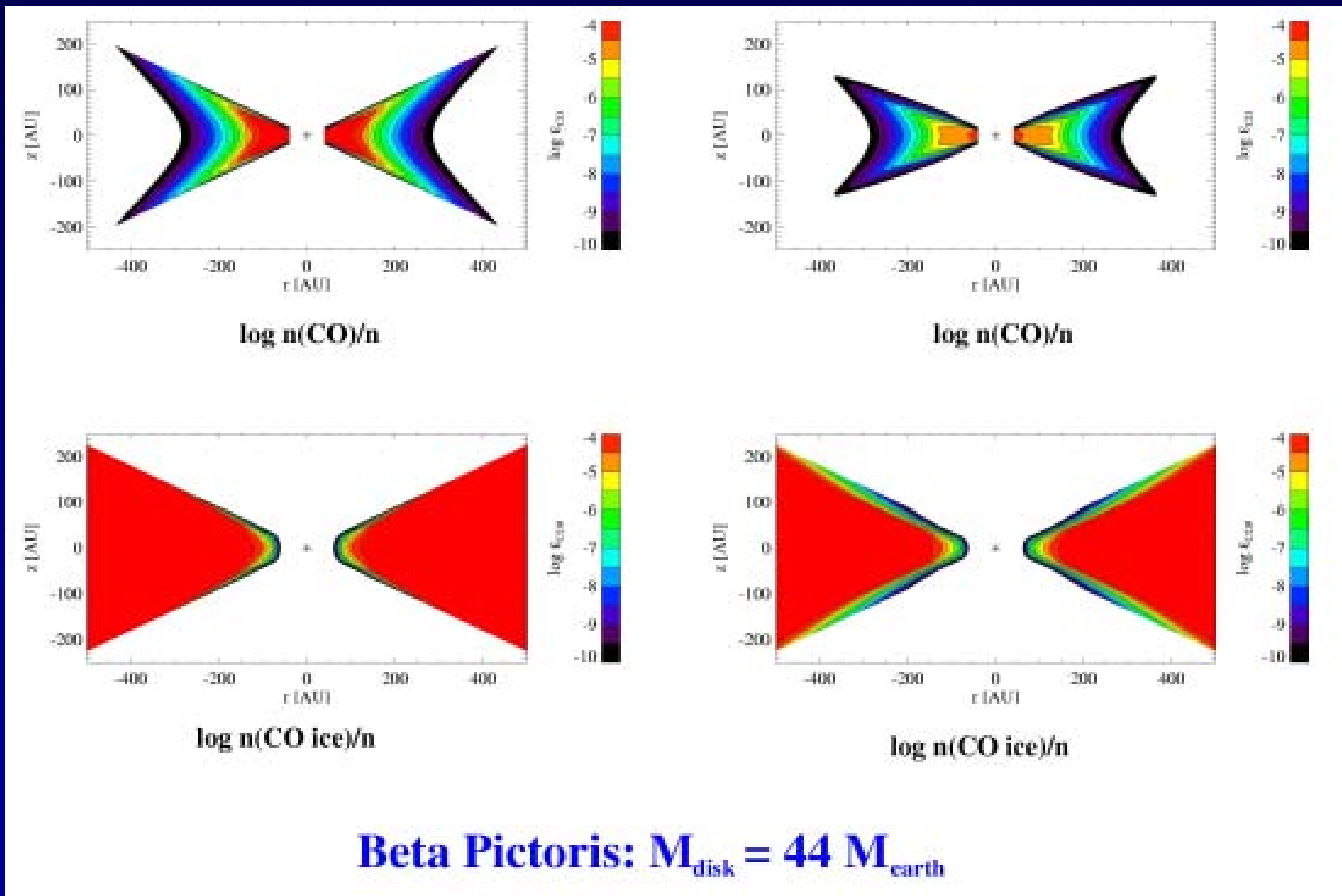
Observational diagnostics stellar UV



- Difficult to disentangle models with single-dish data
- Need ALMA resolution to probe variations
- HCN dissociated by Ly α, CN not

CO gas versus ice

Stellar UV **Stellar + interstellar UV**



CO gas

CO ice

IV. Tenuous disks

- Optically thin: τ<1 in UV continuum (and IR) => analytical solution for T_{dust}
- Typical dust masses: $\sim M_{Earth}$
- Do these disks still contain gas? If so, what is the best tracer?
- Mechanisms for disk dispersal?
  - Accretion onto star, planet formation
  - Stellar wind, photoevaporation, tidal encounters
  - Expect most remaining gas at 10-100 AU